

Université catholique de Louvain ♦ Faculté des sciences

Retrieval of high-altitude temperature profiles from atmospheric limb-scattered radiance

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Use of generative artificial intelligence

*AI is like having a knife. You can use it to cut bread or to hurt someone.
It's up to us to decide how to use it.*

Oren Etzioni, CEO of the Allen Institute for AI

According to the core principles of UCLouvain, any use of generative artificial intelligence (AI) in academic work must be clearly and transparently disclosed. I therefore take this opportunity to specify the role of AI in this Master's thesis.

I did use the OpenAI¹ large language model GPT-5.3 as an assistance tool for translation from French to English and for the rephrasing and revision of parts of this manuscript. In addition, it was used to help structure the Python code employed in the simulations presented throughout the chapters.

The figures, ideas, and bibliographic work in this Master's thesis are my own. I have reviewed and edited the content as needed and I take full responsibility for the content of the thesis.

¹<https://chat.openai.com/>

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Nomenclature

Physical constants

ω	WGS 84 Earth nominal mean angular velocity	$7.292\,115 \times 10^{-5} \text{ rad s}^{-1}$
a	WGS 84 Earth semi-major axis	$6\,378\,137.0 \text{ m}$
b	WGS84 Earth semi-minor axis	$6\,356\,752.3 \text{ m}$
e	WGS 84 Earth first eccentricity	$0.081\,819$
f	WGS 84 Earth flattening	$1/298.257\,223\,563$
G	Gravitational constant	$6.674\,30 \times 10^{-11} \text{ m}^3 \text{ kg}^{-1} \text{ s}^{-2}$
g_0	Gravitational acceleration at the Earth surface	$9.806\,65 \text{ m s}^{-2}$
k_B	Boltzmann constant	$1.380\,649 \times 10^{-23} \text{ J K}^{-1}$
M_{air}	Molar mass of dry air	28.97 g mol^{-1}
M_E	Earth mass	$5.972\,186\,4 \times 10^{24} \text{ kg}$
N_A	Avogadro number	$6.022\,140\,76 \times 10^{23} \text{ mol}^{-1}$
N_s	Molecular number density for standard air	$2.547 \times 10^{19} \text{ cm}^{-3}$
R_E	Earth mean radius	$6\,371\,000.0 \text{ m}$

Radiative quantities

$d\Omega$	Element of solid angle
dA	Element of surface
E	Radiant energy
F	Spectral flux density / spectral irradiance
I	Scalar (spectral) radiance / specific intensity
I_{end}	Scalar (spectral) radiance at path endpoint coordinate
J	Source term
J_1	Single scatter source term

Geometrical quantities

$(\hat{E}, \hat{N}, \hat{U})$	ENU coordinate system axes
$(\hat{x}, \hat{y}, \hat{z})$	ECEF coordinate system axes
(x, y, z)	ECEF Cartesian coordinates
C	Center of curvature
O	Coordinate origin
S	Ellipsoidal surface point
T	Tangent point
α	Normal section azimuth
α_{LOS}	LOS azimuth angle
ϵ	Elevation angle
$\hat{\Omega}$	Unit vector of propagation direction
$\hat{\Omega}_{\odot}$	Unit vector of solar direction
$\hat{n}$	Unit (ellipsoid) normal vector
$\hat{u}$	Unit viewing direction / LOS unit vector
κ	Curvature
λ	Longitude
ϕ	Azimuth angle
$\phi_{\odot}$	Solar azimuth angle
θ	Zenith angle
$\theta_{\odot}$	Solar zenith angle
φ	Geodetic latitude
h	Ellipsoidal height
h_{T}	Tangent altitude
M	Earth's meridional radius of curvature
N	Earth's prime vertical radius of curvature
R	Radius of curvature
$\vec{r}$	3D position vector
$\vec{r}_0$	3D reference (satellite) position vector

s	Path coordinate
s_{end}	Path endpoint coordinate
s_{T}	Tangent path coordinate
Δs	Spatial sampling step

Thermodynamic quantities

C_{CO_2}	CO ₂ concentration
m	Mean molecular mass of air
n	(Volume) Number density
n_{air}	Air (volume) number density
n_{O_3}	Ozone (volume) number density
P	Atmospheric pressure
T	Atmospheric temperature
T_0	Upper boundary (reference) temperature

Optical quantities

λ	Wavelength
ρ	Depolarization factor
σ	Cross section
σ_r	Rayleigh cross section
σ_{O_3}	Ozone cross section
τ	Optical thickness / optical depth
Θ	Scattering angle
F_{K}	King (correction) factor
k	(Total) Extinction coefficient
k_{scatt}	Scattering extinction
k_{abs}	Absorption extinction coefficient
n_s	Refractive index of standard air
p	Phase function
$\bar{p}$	Effective phase function

Retrieval quantities

β	Regularization parameter
γ	Levenberg-Marquardt damping parameter
ξ	Convergence threshold
$\mathcal{J}$	Cost function
$\mathbf{\Gamma}$	Tikhonov regularization matrix
ε	Measurement error vector
$\mathbf{D}$	Levenberg-Marquardt diagonal matrix
$\mathbf{F}$	Forward radiative transfer model
$\mathbf{K}$	Jacobian matrix / weighting function matrix
$\mathbf{L}_2$	Discrete second-derivative operator
$\mathbf{S}_\varepsilon$	Measurement error covariance matrix
$\mathbf{x}$	(Atmospheric) State vector
$\hat{\mathbf{x}}$	(Atmospheric) State vector estimate
$\mathbf{x}_0$	First-guess state vector
$\mathbf{y}$	(Radiance) Measurement vector

Miscellaneous

$\mathcal{R}$	Basis triangular function
g	Local gravitational acceleration
S	Standard deviation
t	Time

Abstract

While the Earth’s surface and the lower part of the atmosphere, the troposphere, are becoming warmer due to the increase in greenhouse gas concentrations, recent observations indicate that the middle atmosphere, the stratosphere and the mesosphere, are cooling. Paradoxically, this cooling is also caused by the increase in long-lived greenhouse gases: they broadly reradiate their energy which, from the higher atmosphere, can escape to outer space. Monitoring the cooling of the upper atmosphere is another important component of the global efforts to track the anthropogenic climate change.

The Limb Profiler (LP) instrument of the Ozone Mapper and Profiler Suite (OMPS) measures the radiance of the atmospheric limb during the day. It observes the limb-scattered solar light from the ultraviolet to the near-infrared domain (approximately 290–1000 nm). With the help of a model of the light-atmosphere interaction (a radiative transfer model, RTM), profiles of the atmospheric composition can be inferred with a vertical resolution of approximately 2 km.

In this Master’s thesis, an RTM is developed to describe the propagation of solar radiation in a spherical-shell atmosphere, assuming that photons are scattered only once before reaching the detector (single-scattering approximation). This approximation is justified by the low air number density in the middle atmosphere compared to the troposphere, which makes multiple scattering negligible over the altitude range considered (approximately 35–80 km). The model is implemented in Python and validated against the reference RTM SASKTRAN. The validated model is then used to process the OMPS-LP observations, considering Rayleigh scattering as the sole scattering process and accounting only for extinction by Rayleigh scattering and ozone absorption. Atmospheric number density profiles are retrieved using a standard inverse retrieval scheme, from which temperature profiles are derived using the combination of the hydrostatic equilibrium equation and the ideal gas law.

Chapter 1

Introduction

The global cooling effect

The atmosphere is essential to life on Earth. It supplies the oxygen required for breathing, allows water to remain liquid in the oceans, and acts as a shield against harmful solar radiation. The atmosphere also helps to keep the surface of the Earth warm by trapping some of the outgoing thermal radiation in a process called the *greenhouse effect*. Without it the average temperature of the Earth's surface would be much lower, around -18°C , compared to the current global average of about 15°C [1].

The Earth's atmosphere is made up of several distinct layers. This stratification comes from the particular variation of temperature with altitude. Unlike air pressure and density, which decrease approximately exponentially with altitude, the temperature in the atmosphere has a much more complex vertical profile, as illustrated in Figure 1.1. The lowest layer is the *troposphere*, extending from the surface up to about 15 km high and containing about 85–90% of the atmosphere's mass. It is characterized by a decrease in temperature with increasing altitude because it is primarily heated from the Earth's surface. Above the troposphere lies the *stratosphere*, which goes from about 15 to 50 km high. In this layer, temperature increases with altitude due to the absorption of solar ultraviolet (UV) radiation by the ozone layer. The next layer is the *mesosphere*, ranging from 50 to 90 km high, where temperatures once again decrease with height up to -90°C , making it the coldest part of the atmosphere. The *thermosphere* is the fourth layer, where temperature increases steadily with altitude because it is directly exposed to strong solar radiation. Finally, there is the *exosphere*, which is the outermost layer where the atmosphere progressively merges into outer space.

The present work focuses on temperatures in the upper stratosphere and mesosphere, regions commonly grouped under the name of *middle atmosphere*. Below 30 km, the term *lower atmosphere* will be used, while the region beyond the mesosphere will be referred to as the *upper atmosphere*.

The temperature profile presented in Figure 1.1 represents only an average state of the atmosphere, since atmospheric temperature varies not only with altitude but also temporally. There is now unequivocal evidence that the Earth is warming. Over recent decades, surface temperatures have increased due to climate change driven by the growing concentration of greenhouse gases emitted by human activities [3, 4]. The theoretical basis for this warming was first established by climatologists Syukuro Manabe and Richard Wetherald in 1966 [5]. Using a simplified general

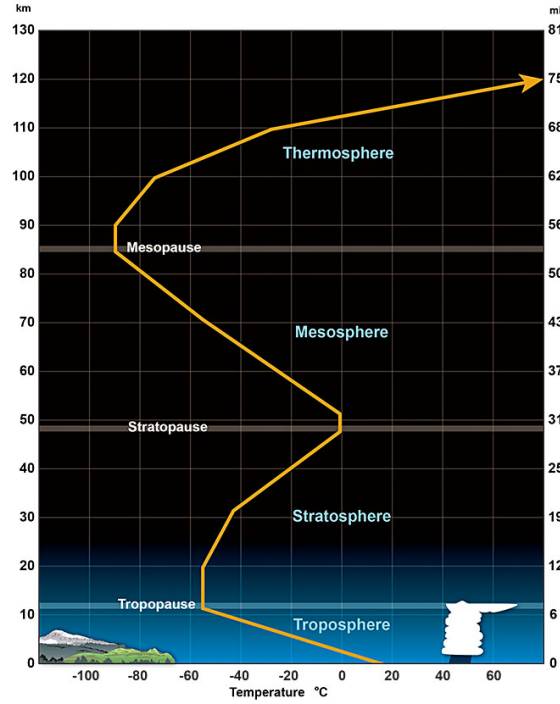


Figure 1.1: Average temperature profile of the Earth’s atmosphere showing the main atmospheric layers (from [2]).

circulation model, they demonstrated that doubling the atmospheric concentration of carbon dioxide (CO_2) leads to a global warming of approximately 2°C at the Earth’s surface and within the troposphere.

However, the thermal response to increasing CO_2 concentrations is not the same throughout the atmosphere. While greenhouse gases warm the surface and lower atmosphere by trapping outgoing infrared (IR) radiation, they induce a cooling effect in the middle atmosphere [6]. The middle atmosphere is much less dense than the lower atmosphere, making it much more transparent to outgoing IR radiation. Consequently, as CO_2 concentrations increase, more IR radiation is emitted to space. This *cooling-to-space effect* ultimately results in a decrease in temperature in the middle and upper atmosphere [7]. Continuous long-term observations of middle atmospheric temperatures are therefore essential for assessing the consequences of both natural and anthropogenic changes in CO_2 concentrations in this region.

Temperature measurements

The atmospheric sounding of the temperature can be performed either directly through in situ observations or indirectly using remote sensing techniques.

In situ measurements are obtained using instruments placed directly within the atmospheric region being studied. A common example is the *radiosonde*, which is carried aloft by weather balloons and is equipped with sensors that can measure the atmospheric temperature during ascent. Currently, radiosonde observations from approximately 1000 active stations worldwide are assimilated into numerical weather prediction models¹. Due to their high vertical resolution, typically of the order of a

¹The Royal Meteorological Institute of Belgium performs radiosonde launches three times per week in Uccle [8].

few meters, radiosonde measurements play a central role in modern meteorology [9]. However, as the balloon ascends into the atmosphere, the decreasing pressure causes it to expand until it eventually explodes. As a consequence, radiosonde observations are generally limited to altitudes below approximately 30 km, whereas this study focuses on temperatures at higher altitudes.

For this reason, indirect methods based on *remote sensing* are well suited for studying the middle atmosphere. Satellite-based remote sensing techniques provide global, frequent, and repetitive observations of the atmosphere. Rather than directly measuring temperature as a thermometer attached to a radiosonde would, instruments onboard satellites, such as *spectroradiometers*, detect electromagnetic radiation emitted or scattered by the atmospheric constituents over a broad range of wavelengths. More specifically, satellite sensors measure a quantity known as *radiance*, which corresponds to the radiant flux received within a given spectral range. Since the interaction of radiation with the atmosphere depends on the composition and thermodynamic state of the atmospheric layers, these radiance measurements can be used to infer the temperature and chemical composition through retrieval techniques.

Observation geometries

Most satellite temperature measurements rely on two main observation geometries: *nadir-viewing* and *limb-viewing*.

In nadir-viewing geometry, instruments observe the atmosphere by looking directly downward toward the Earth’s surface (Figure 1.2). Between 1979 and 2006, the Stratospheric Sounding Unit (SSU) instruments provided long-term temperature measurements in the stratosphere using a three-channel IR radiometer [10]. The Version 2 SSU temperature time series revealed global stratospheric cooling trends from approximately -0.69 K/decade to -0.85 K/decade depending on altitude, in agreement with chemistry-climate model simulations. Moreover, since 1998, the Advanced Microwave Sounding Unit (AMSU) sensors have measured upwelling microwave radiation emitted by atmospheric oxygen. Thanks to their finer vertical resolution compared to SSU observations, AMSU measurements have been used to infer atmospheric temperatures and investigate regional and seasonal cooling trends in the middle atmosphere during the 2002–2014 period [11]. This study confirmed that the global cooling of the stratosphere continued over this period, with cooling rates from -0.4 to -0.5 K/decade above 25 km. However, nadir-viewing observations generally suffer from a relatively poor vertical resolution of 5–10 km.

Limb-viewing observations, on the other hand, provide an improved vertical resolution of approximately 2–3 km. In this geometry, the line of sight (LOS) of the instrument follows a nearly tangential path through the Earth’s atmosphere (Figure 1.2), successively probing different altitude layers. Limb-viewing techniques can generally be divided into two categories: *occultation measurements* and *limb-scatter observations*.

In solar or stellar occultation measurements, the instrument continuously monitors the attenuation of radiation emitted by the Sun or a star as it passes through the atmosphere. From a satellite platform, the Sun rises and sets through the atmosphere once per orbit. The number of measurements per orbit is therefore limited, resulting in reduced spatial coverage with solar occultation. Nevertheless, the Global Ozone Monitoring by Occultation of Stars (GOMOS) instrument enabled temper-

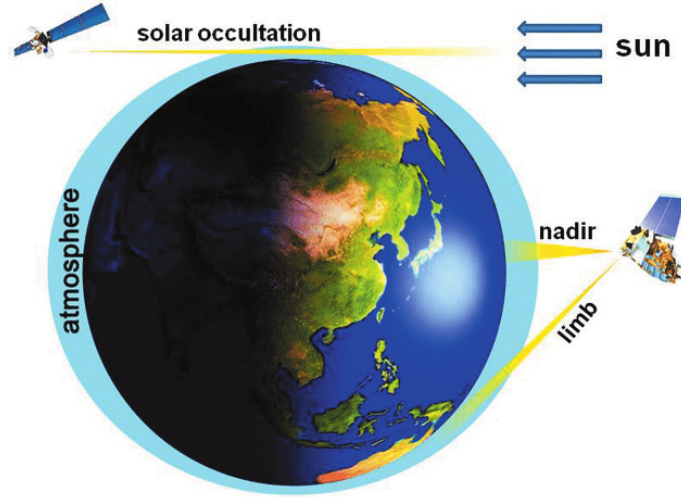


Figure 1.2: Illustration of the two main satellite observation geometries used in atmospheric remote sensing. In nadir-viewing geometry, the instrument is looking straight down, whereas in limb-viewing geometry, the line of sight passes nearly tangentially through the atmosphere (from [12]).

ature retrievals with a vertical resolution of approximately 2 km between 35 and 85 km altitude using stellar occultation [13].

In the case of limb-scatter observations, the instrument observes sunlight scattered by atmospheric constituents along the LOS. Limb-scatter measurements combine two major advantages: a vertical resolution comparable to that of occultation techniques and a good global coverage similar to nadir sounding. However, the long optical path through the atmosphere also increases the complexity of the radiative transfer processes involved. Several studies have demonstrated the capability of retrieving stratospheric and mesospheric temperature profiles from limb sounder observations. The first demonstration of upper-stratospheric temperature retrieval using limb-scattered radiation was achieved with the visible-light spectrometer onboard the Solar Mesosphere Explorer (SME) satellite [14]. More recently, Zawada et al. [15] and Sheese et al. [16] used limb-scattered spectra measured by the Optical Spectrograph and InfraRed Imaging System (OSIRIS) to retrieve upper-stratospheric (35–60 km) and mesospheric (55–80 km) temperature profiles, respectively. Furthermore, among current limb-scatter instruments, the Ozone Mapping and Profiler Suite Limb Profiler (OMPS-LP) provides continuous global observations of the middle atmosphere in the UV-visible spectral range. Recent studies have demonstrated the feasibility of retrieving upper-stratospheric and mesospheric temperature profiles from OMPS-LP limb-scattered radiances near 350 nm [17, 18].

Since satellite missions have a limited duration, long-term temperature trends are generally obtained by combining datasets from multiple instruments and observation techniques. For instance, Randel et al. [19] combined observations from SSU, the Aura Microwave Limb Sounder (MLS), and the Sounding of the Atmosphere Using Broadband Emission Radiometry (SABER) instrument to investigate stratospheric temperature trends between 1979 and 2015. Their results highlighted a long-term cooling, the magnitude of which increases with altitude, ranging from -0.1 to -0.2 K/decade in the lower stratosphere to -0.5 to -0.6 K/decade in the middle and upper stratosphere. Furthermore, Dubé et al. [20] reported a cooling

rate of approximately -0.6 K/decade near 45 km between 1979 and 2021 by combining SSU and OSIRIS observations. They also showed that the cooling rate is slightly greater in the Northern Hemisphere than in the Southern Hemisphere.

Stratospheric data deficit

Despite its importance for climate studies, the middle atmosphere remains a region less explored than the lower atmosphere. This lack of observations can introduce biases in atmospheric reanalysis products such as ERA5, which are widely used in climate projection systems [21]. In the future, this could also cause significant problems for climate models to accurately represent the radiative coupling between atmospheric layers of the atmosphere, as modern climate models increase their vertical resolution and extend their upper boundaries into the mesosphere [22].

The situation may worsen in the coming years, as the scientific community is currently facing a critical data deficit in the stratosphere [23]. Indeed, only a limited number of upcoming satellite missions are specifically designed to continue monitoring the middle atmosphere, notably the Joint Polar Satellite System (JPSS) satellites carrying the OMPS-LP instrument [24], as well as the upcoming Atmospheric Limb Tracker for the Investigation of the Upcoming Stratosphere (ALTIUS) mission [25], initiated at the Royal Belgian Institute for Space Aeronomy (BISA).

Objectives and strategy

In this context, this Master’s thesis proposes to (i) construct a *radiative transfer model* (RTM) based on the single-scattering approximation and (ii) develop a temperature retrieval algorithm and apply it to recent limb-scattered radiance data from OMPS-LP.

Accurate modeling of the various physical processes affecting the propagation of solar radiation requires the use of a RTM. This forward model is first required to simulate limb-scattered radiances for a specified atmospheric state. Many RTMs have been developed for limb-scattering applications, including Siro [26], LIMBTRAN [27], Gauss–Seidel limb scattering (GSLs) [28], and SASKTRAN [29] models. Although these models are extremely versatile and can generally be adapted to different observation geometries and multiple-scattering simulations, this often comes with a significant computational burden.

The present work therefore focuses on the development of a simplified RTM based on the single-scattering approximation and optimized for limb-scatter temperature retrievals. This RTM represents a first step toward future applications for the bright limb observation mode of the ALTIUS mission. The theoretical development of the model is presented in Chapter 2, where the radiative transfer equation in a spherical atmosphere is introduced together with its solution under the single-scattering approximation. Chapter 3 then describes the numerical implementation of the different stages of the calculation and the practical computation of limb-scattered radiance profiles. The model is subsequently validated through comparisons with SASKTRAN model.

The second part of this work focuses on the inversion algorithm used to retrieve atmospheric temperature profiles from limb-scattered radiances. Above 30 km, scattering of sunlight in the UV and visible spectral regions is dominated by Rayleigh

scattering from atmospheric molecules. Since the intensity of elastic Rayleigh scattering is directly proportional to atmospheric density, it is thus possible to retrieve air density profiles from limb-scattered radiance measurements. Combined with the hydrostatic equilibrium equation and the ideal gas law, these density profiles can then be used to derive absolute temperature profiles. Chapter 4 therefore presents the temperature retrieval algorithm developed in this work together with its validation using simulated observations. The retrieval method is finally applied to recent OMPS-LP limb-scatter measurements.

Chapter 2

Radiative transfer model

A *radiative transfer model* (RTM) aims to provide the most accurate possible representation of the physical processes governing the transport of energy in the form of electromagnetic radiation. It is used to describe the propagation of radiation through a planetary atmosphere, accounting for absorption, emission, and scattering processes. The primary purpose of such a model is to establish a quantitative link between satellite observations and the atmospheric state. Consequently, the accuracy of the retrieved atmospheric parameters, obtained through the inversion procedure described in Chapter 4, directly depends on the accuracy of the model.

Throughout this chapter, the theoretical development of radiative transfer is introduced. The geometric framework and coordinate systems required to describe the limb observation geometry are also presented. The model formulation, its inputs, and its main assumptions are finally summarized to bridge the gap to the next chapter.

2.1 Radiative transfer theory

In this section, the radiative transfer theory is presented in detail in order to introduce the theoretical framework underlying the RTM developed in this work. The propagation of radiation through a planetary atmosphere is mathematically described by the *radiative transfer equation*, originally formalized by the co-winner of the 1983 Nobel Prize in Physics, Subrahmanyan Chandrasekhar [30]. For the sake of clarity, more modern notations taken from [31] will be used throughout this section.

2.1.1 Description and definitions

The fundamental quantity describing a radiation field at position $\vec{r}$ and propagating in a direction specified by the unit vector $\hat{\Omega}$ is the *spectral radiance* (also referred to as

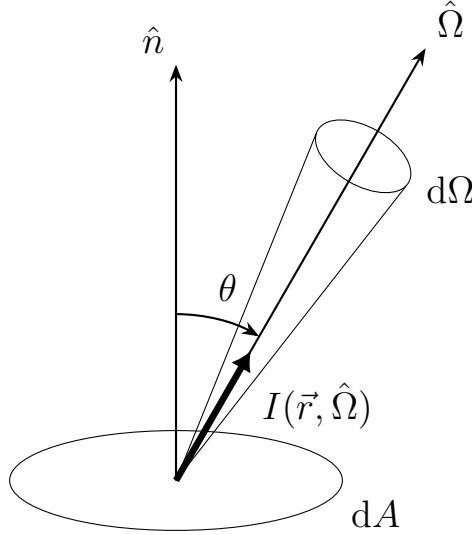


Figure 2.1: The spectral radiance $I(\vec{r}, \hat{\Omega})$ is defined at position $\vec{r}$ in the direction $\hat{\Omega}$ within the solid angle $d\Omega$. Radiation is emitted (or received) by a surface element dA with normal $\hat{n}$. The angle between $\hat{n}$ and $\hat{\Omega}$ is denoted by θ . This construction also defines a *pencil of radiation* or a *radiation beam*.

the *specific intensity*), denoted $I_\lambda(\vec{r}, \hat{\Omega})^1$. It is defined as the radiant energy $dE_\lambda(\vec{r})$, within a wavelength interval $(\lambda, \lambda + d\lambda)$, transported through a surface element dA in directions within a solid angle element $d\Omega$ during a time dt ,

$$I_\lambda(\vec{r}, \hat{\Omega}) = \frac{dE_\lambda(\vec{r})}{dt dA \cos \theta d\lambda d\Omega}, \quad (2.1)$$

where the angle θ is defined between the propagation direction $\hat{\Omega}$ and the surface normal $\hat{n}$, as shown in Figure 2.1. The SI unit of spectral radiance is $\text{W m}^{-2} \text{sr}^{-1} \text{nm}^{-1}$.

In addition to radiance, a complete description of the radiation field requires the specification of its *polarization state*. The polarization of light characterizes the orientation of its oscillations². For instance, sunlight is said to be unpolarized, as its oscillations vary randomly without any preferred orientation, whereas an initially unpolarized beam may become partially polarized after experiencing scattering. In the present work, polarization effects will no longer feature in the description of the RTM.

The *spectral flux density* $F(\vec{r}, \hat{n})$, also referred to as *spectral irradiance*, can be defined as the integral of the projection of the radiance onto the surface normal $\hat{n}$

¹For simplicity, the spectral dependence (the index λ) will be omitted in the following, and $I(\vec{r}, \hat{\Omega})$ will denote the radiance, even if, strictly speaking, the *radiance* is the *integrated intensity* defined as the integral of spectral radiance over the entire wavelength spectrum,

$$I(\vec{r}, \hat{\Omega}) = \int_0^\infty I_\lambda(\vec{r}, \hat{\Omega}) d\lambda.$$

From now on, all quantities are considered monochromatic.

²An electromagnetic wave such as light consists of a coupled oscillating electric field and magnetic field that are always perpendicular to each other.

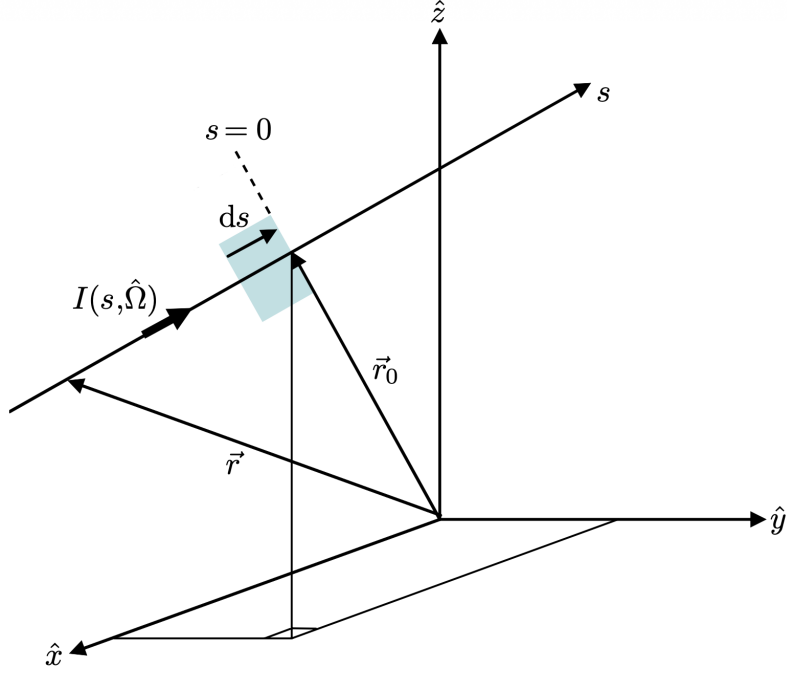


Figure 2.2: A radiation beam with radiance $I(s, \hat{\Omega})$ propagates in direction $\hat{\Omega}$ along increasing path coordinate s . The point labeled $s = 0$ denotes a reference location, and ds is an infinitesimal path length element in the propagation direction (adapted from Figure 4.3 in [31]).

over the solid angle of the incoming hemisphere,

$$F(\vec{r}, \hat{n}) = \int_{2\pi} I(\vec{r}, \hat{\Omega}') \cos \theta' d\Omega', \quad (2.2)$$

where θ' is the angle between $\hat{\Omega}'$ and $\hat{n}$. Its SI unit is $\text{W m}^{-2} \text{nm}^{-1}$.

While this formulation specifies the radiation field at a given spatial position $\vec{r}$ and in a direction, it is essential to describe how radiation evolves as it propagates through a medium. Assuming that radiation in the Earth's atmosphere travels in a straight line³, it is useful to parameterize the transport path using a *geometric path coordinate* s such that

$$\vec{r} = \vec{r}_0 + \hat{\Omega}s, \quad (2.3)$$

where $\vec{r}_0$ is a reference point. In this work, $\vec{r}_0$ corresponds to the observation point (satellite location), and the path coordinate is defined such that $s = 0$ at the observer. The radiance is thus written in terms of the path coordinate only, that is,

$$I(s) \equiv I(s, \hat{\Omega}) \equiv I(\vec{r}, \hat{\Omega}). \quad (2.4)$$

This is illustrated in Figure 2.2.

³This is not generally the case due to *atmospheric refraction*. As the refractive index of the atmosphere varies with altitude, light traveling through the atmosphere is “deflected” and thus follows a curved path. However, refraction effects are assumed to be negligibly small, as this study focuses on the middle atmosphere, where air density is low.

2.1.2 Radiative transfer equation

Beer–Lambert law

As radiation propagates through a medium, it is attenuated due to absorption and scattering processes involving the various species composing that medium. The degree of attenuation depends on both the number of interacting particles and their interaction strength. More formally, when a beam of radiation travels through an infinitesimally thin region of thickness ds , along the direction of propagation $\hat{\Omega}$, the radiance $I(s)$ follows the Beer–Lambert law,

$$\frac{dI(s)}{ds} = -I(s) \sum_i \sigma_i(s) n_i(s), \quad (2.5)$$

where dI is the change in radiance due to an interaction with atmospheric species i that attenuates the incident radiation through absorption and/or scattering processes. The *species cross section* σ_i quantifies the likelihood of interaction between the particles of the beam and the particles of the species i in units of area (m^2). Although not explicitly stated here, the cross section depends on the wavelength (see footnote 1). The *species (volume) number density* n_i , expressed in m^{-3} , is the number of particles of the species i per unit volume. These last two quantities generally depend on the position along the propagation path s in the atmosphere.

Equation (2.5) can be rewritten as

$$\frac{dI(s)}{ds} = -k(s)I(s), \quad (2.6)$$

by introducing the *extinction coefficient*

$$k(s) = \sum_i \sigma_i(s) n_i(s), \quad (2.7)$$

characterizing the total extinction caused by the individual species that make up the atmosphere. It should be noted that the extinction coefficient is the inverse of the mean free path, and therefore its units are those of an inverse length (m^{-1}).

This extinction coefficient can naturally be broken down into two components: a component $k_{\text{scatt}}(s)$ related to scattering processes and another component $k_{\text{abs}}(s)$ related to absorption processes,

$$k(s) = k_{\text{scatt}}(s) + k_{\text{abs}}(s). \quad (2.8)$$

The radiance at any point along the path is determined by rearranging and integrating (2.6) from s to the reference point $s = 0$,

$$\int_{I(s)}^{I(0)} \frac{dI(s')}{I(s')} = - \int_s^0 k(s') ds'. \quad (2.9)$$

The *optical thickness* τ (or *optical depth*) is a dimensionless measure of radiation attenuated in a medium. More specifically, it corresponds to the integral of the extinction along the path traveled by the beam,

$$\tau(s_1, s_2) = \int_{s_1}^{s_2} k(s) ds, \quad (2.10)$$

between any two points s_1 and s_2 . The limits $\tau \ll 1$ ($\tau \gg 1$ respectively) are called *optically thin* (*optically thick* respectively).

In the case of a homogeneous layer of thickness l , that is, a layer for which the extinction coefficient k does not depend on the path coordinate s , the optical thickness is simply the product $\tau = kl$.

Hence, the radiance observed at the reference point can be expressed in terms of the radiance at any point along the path s and the optical thickness $\tau(s, 0)$ between that point and the reference as

$$I(0) = I(s)e^{-\tau(s,0)}. \quad (2.11)$$

Thus, the larger the optical thickness, the smaller the amount of radiation transmitted through the medium.

Source term

Up to this point, only the attenuation of radiation due to extinction processes (absorption and scattering out of the propagation direction) has been considered. However, radiation can also be scattered from other directions into the propagation direction, thereby increasing the radiance along the path. More generally, three physical processes can contribute to such an increase in radiance in the atmosphere: scattering of radiation into propagation direction, thermal emission of blackbody radiation, and photochemical emission. In the shortwave spectral range ($\lambda < 2 \mu\text{m}$), radiance is dominated by solar radiation scattered by the atmosphere and the surface, while terrestrial thermal emission is negligible [31]. Photochemical emission (e.g. airglow), which primarily occurs in the middle atmosphere, can also be neglected in this regime. In the present work, the source term is therefore assumed to arise solely from scattering processes. This corresponds to the assumption of a *scattering atmosphere*.

To account for both the negative and positive contributions of the change in radiance along the direction of propagation, a *source term* $J(s)$ is introduced into the Beer–Lambert equation (2.6), resulting in the *integro-differential form of the radiative transfer equation*,

$$\frac{dI(s)}{ds} = k(s)(-I(s) + J(s)). \quad (2.12)$$

This equation (2.12) simply states that, as radiation propagates through the medium, it loses energy through extinction processes and gains energy through contributions from other directions.

For a scattering atmosphere, the source term is expressed as an integral of the diffuse radiance over all directions scattered into the propagation direction,

$$J(s, \hat{\Omega}) = \frac{k_{\text{scatt}}(s)}{k(s)} \frac{1}{4\pi} \int_{4\pi} I(s, \hat{\Omega}') p(s, \Theta) d\Omega'. \quad (2.13)$$

Here, the radiance $I(s, \hat{\Omega}')$ is explicitly written as a function of the direction $\hat{\Omega}'$ to highlight that the diffuse radiance over all directions can be scattered into the direction $\hat{\Omega}$. The term $p(s, \Theta)$ is called the *phase function*, which characterizes the angular distribution of scattered radiation. It defines the probability per unit solid

angle that radiation propagating in direction $\hat{\Omega}'$ is scattered into direction $\hat{\Omega}$. The phase function is normalized such that

$$\frac{1}{4\pi} \int_{4\pi} p(s, \Theta) d\Omega' = 1. \quad (2.14)$$

The angle Θ is the *scattering angle*, defined as the angle between the incoming and outgoing directions, i.e., between the diffuse radiance direction and the propagation direction,

$$\cos \Theta = \hat{\Omega} \cdot \hat{\Omega}'. \quad (2.15)$$

The integro-differential radiative transfer equation (2.12) can be transformed into a more intuitive integral form,

$$I(0) = I(s)e^{-\tau(s,0)} + \int_s^0 k(s')J(s')e^{-\tau(s',0)}ds'. \quad (2.16)$$

This expression states mathematically that the radiance observed at the reference point $s = 0$ is composed of two contributions: the radiance originating from the end of the path, $I(s)$, attenuated to the observer by the factor $e^{-\tau(s,0)}$, and the cumulative contribution of the scattered source term along the path, also appropriately attenuated back to the observer by the factor $e^{-\tau(s',0)}$.

2.2 Radiative processes

The term *radiative processes* encompasses all physical mechanisms responsible for the transfer of energy through a medium in the form of electromagnetic radiation. It has previously been established, in Subsection 2.1.2, that a multi-component medium such as the Earth's atmosphere can absorb, emit, and scatter radiation. The relative importance of these processes is strongly dependent on wavelength. In the present work, only two mechanisms are considered: Rayleigh scattering and ozone (O_3) absorption.

2.2.1 Rayleigh scattering

Rayleigh scattering is a process in which electromagnetic radiation is elastically scattered by atmospheric particles whose characteristic size is much smaller than the wavelength of the incident radiation. The process is classified as elastic since the wavelength of the scattered light and the incident light are identical. Named after Lord Rayleigh (John William Strutt), this mechanism is the dominant molecular scattering in a clear atmosphere [32]. In the Earth's atmosphere, it arises mainly from interactions with atmospheric gases such as nitrogen (N_2), oxygen (O_2), and other trace gases. In 1871, Lord Rayleigh showed that the scattering intensity varies inversely with the fourth power of wavelength, explaining the strong wavelength dependence of atmospheric scattering and, in particular, the blue color of the sky [33].

The *total Rayleigh scattering cross section per molecule of air* $\sigma_r(\lambda)$ quantifies the efficiency with which a particle scatters incident radiation and is given by:

$$\sigma_r(\lambda) = \frac{24\pi^3(n_s^2 - 1)^2}{\lambda^4 N_s^2(n_s^2 + 2)^2} \left[\frac{6 + 3\rho}{6 - 7\rho} \right], \quad (2.17)$$

where the wavelength λ is expressed in cm. The different parameters appearing in this expression are detailed below.

The *molecular number density for standard air* N_s is derived from standard pressure (101 325 Pa) and temperature (288.15 K) at the surface:

$$N_s = \frac{101\,325}{288.15\,k_B} \approx 2.547 \times 10^{19} \text{ cm}^{-3}, \quad (2.18)$$

where $k_B = 1.380\,649 \times 10^{-23} \text{ J K}^{-1}$ is the Boltzmann constant.

The *refractive index of standard air* n_s has been extensively studied during the second half of the 20th century due to its wavelength dependence. *Standard air* is defined as dry air containing 0.03% carbon dioxide (CO_2)⁴ by volume at normal pressure and temperature. Several empirical formulations exist, typically expressed in terms of $(n_s - 1)$ since the refractive index of air is very close to unity. Here, we use the Peck and Reeder's 1972 formula [34], which refines Edlén's 1966 expression [35] using updated experimental data, is preferred:

$$(n_s - 1)_{300} \times 10^8 = 8060.51 + \frac{2\,480\,990}{132.274 - \lambda^{-2}} + \frac{17\,455.7}{39.329\,57 - \lambda^{-2}}, \quad (2.19)$$

where the wavelength is expressed in μm and the subscript 300 indicates that the formula is valid for air containing 300 ppm CO_2 . This expression is valid over the spectral range $\lambda \in [0.185 \mu\text{m}, 1.69 \mu\text{m}]$.

In the present work, following the recommendation of Bodhaine [36], the Peck and Reeder's formulation for dry air with 300 ppm CO_2 is adapted to account for the actual CO_2 concentration C_{CO_2} using the relation from [35]:

$$\frac{(n_s - 1)_{C_{\text{CO}_2}}}{(n_s - 1)_{300}} = 1 + 0.54(C_{\text{CO}_2} - 0.0003), \quad (2.20)$$

where the CO_2 concentration is expressed as parts per volume. In this work, the CO_2 concentration is assumed to be $C_{\text{CO}_2} = 360 \text{ ppm} = 0.036\% = 0.00036$.

Finally, the term $(6 + 3\rho)/(6 - 7\rho)$ in equation (2.17) is known as the *King (correction) factor* F_K , where ρ is the *depolarization factor* accounting for molecular anisotropy. Bates was among the first to account for this spectral dependence based on laboratory measurements and theoretical considerations [37]. He computed wavelength-dependent King factors as the weighted sum of the contributions due to the main atmospheric constituents, namely N_2 , O_2 , argon (Ar), and CO_2 , each weighted by its volume concentration and specific spectral behavior. The King factor for air is then expressed as:

$$F_K(\text{air}) = \frac{78.084 F_K(\text{N}_2) + 20.946 F_K(\text{O}_2) + 0.934 F_K(\text{Ar}) + C_{\text{CO}_2} F_K(\text{CO}_2)}{78.084 + 20.946 + 0.934 + C_{\text{CO}_2}}, \quad (2.21)$$

where C_{CO_2} is expressed as a volume percentage (0.036 for 360 ppm). Bates provided the following expressions for the individual contributions [37]:

$$F_K(\text{N}_2) = 1.034 + 3.17 \times 10^{-4} \lambda^{-2}, \quad (2.22)$$

$$F_K(\text{O}_2) = 1.096 + 1.385 \times 10^{-3} \lambda^{-2} + 1.448 \times 10^{-4} \lambda^{-4}, \quad (2.23)$$

$$F_K(\text{Ar}) = 1.00, \quad (2.24)$$

$$F_K(\text{CO}_2) = 1.15. \quad (2.25)$$

⁴In this work, standard air is assumed to contain 300 parts-per-million (ppm) CO_2 .

Both Bates and Bodhaine neglect dispersion effects due to other atmospheric constituents such as water vapor [36, 37]. This is justified because water vapor is typically confined to the lower troposphere, which complicates the calculation, whereas CO₂ is well mixed throughout the atmosphere. As a consequence, the King factor $F_K(\text{air})$ is considered independent of altitude.

Combining all terms yields the total Rayleigh scattering cross section, which directly enters the definition of the scattering extinction coefficient k_{scatt} . This coefficient is defined as the product of the air number density $n_{\text{air}}(h)$ and the Rayleigh cross section σ_r :

$$k_{\text{scatt}}(h) = \sigma_r n_{\text{air}}(h), \quad (2.26)$$

where the dependence on wavelength is implicit, as well as the dependence on the path parameter s through $h = h(s)$.

The final characteristic of Rayleigh scattering is its phase function $p(\Theta)$, which depends only on the cosine of the scattering angle Θ through [30]:

$$p(\Theta) = \frac{3}{4} (1 + \cos^2 \Theta). \quad (2.27)$$

This function satisfies the normalization condition (2.15) and corresponds to a *conservative scattering case*. Rayleigh scattering enhances forward ($\Theta = 0^\circ$) and backward ($\Theta = 180^\circ$) directions as shown in Figure 2.3.

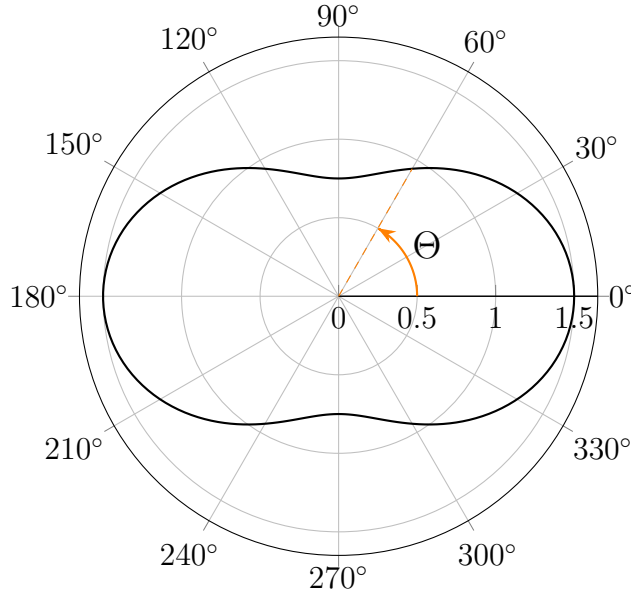


Figure 2.3: Polar representation of the Rayleigh phase function (2.27) showing the angular distribution of scattered radiation as a function of the scattering angle Θ .

2.2.2 Ozone absorption

In the UV-visible spectral range considered in this work, ozone is the dominant absorbing species in the Earth's atmosphere. Its radiative impact is therefore explicitly accounted for in the RTM through its wavelength-dependent absorption cross section $\sigma_{\text{O}_3}(\lambda)$, which also exhibits, to a lesser extent, a temperature dependence. The

ozone absorption cross section spectrum has been extensively measured in the laboratory and is available across a wide spectral range, as illustrated in Figure 2.4 based on measurements by Burrows et al. [38].

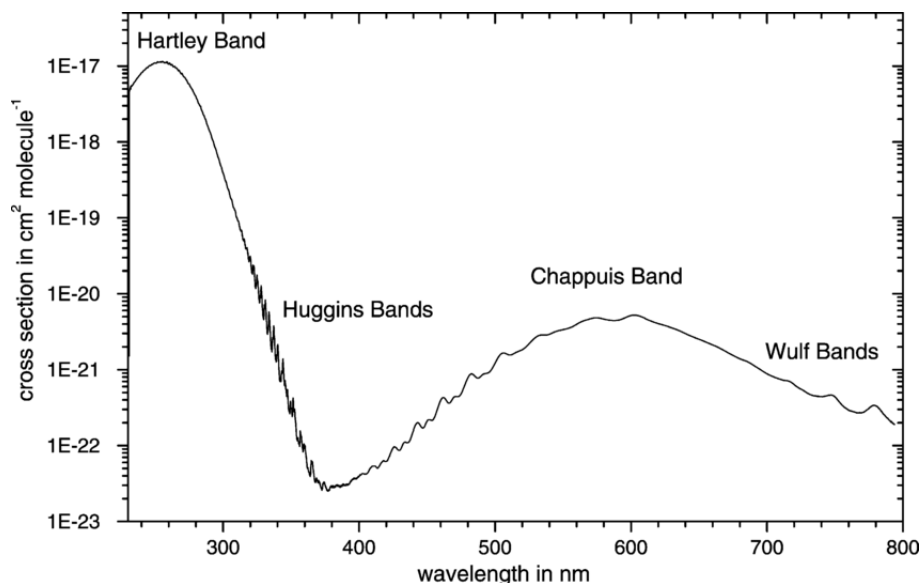


Figure 2.4: Ozone absorption cross section spectrum at 293 K in the 231–794 nm range (from [39]).

The ozone absorption spectrum in the 240–790 nm range is conventionally divided into four main bands: the Hartley, Huggins, Chappuis, and Wulf bands (see Figure 2.4). The *Hartley band* (200–320 nm) is the strongest band, with a maximum around 255 nm, and dominates the absorption of solar UV radiation in the atmosphere. The *Huggins bands* (300–390 nm) consist of a series of individual peaks with a strong temperature dependence. The *Chappuis band* (approximately 390–800 nm) is a broad and relatively weak absorption band in the visible range, with cross sections typically three orders of magnitude smaller than those of the Hartley band. Finally, the *Wulf bands* extend further into the near-IR with very weak absorption.

Ozone is a minor constituent of the atmosphere but plays a crucial role in the Earth’s radiative balance. As shown schematically in Figure 2.5, it is primarily located in the stratosphere, between approximately 15 and 40 km altitude, where it forms the so-called *ozone layer*. This layer results from the photochemical balance described by the Chapman cycle, involving the photodissociation of molecular oxygen and the subsequent formation and destruction of ozone.

The ozone layer efficiently absorbs incoming solar UV radiation, in particular in the UV-C spectral region. This absorption strongly reduces the UV flux reaching the Earth’s surface and thereby protects living organisms from harmful radiation, including DNA damage. It is also important to note that the ozone layer is sensitive to anthropogenic perturbations. The depletion of stratospheric ozone, especially over Antarctica (the so-called *ozone hole*), is primarily driven by catalytic destruction cycles involving halogen radicals released from chlorofluorocarbons.

In contrast, ozone in the troposphere, often referred to as *bad ozone*, acts as a pollutant (see Figure 2.5). It is formed by photochemical reactions involving mainly nitrogen oxides. Unlike stratospheric ozone, tropospheric ozone has harmful effects on human health and vegetation. Its concentration has increased significantly since

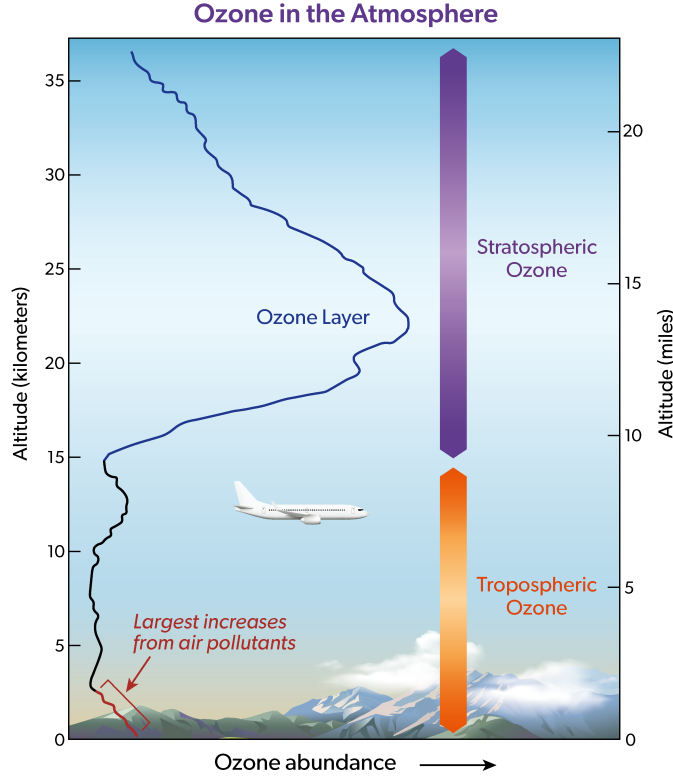


Figure 2.5: Schematic vertical profile of O_3 abundance in the Earth’s troposphere and stratosphere, highlighting the stratospheric ozone layer and the tropospheric bad ozone (from [40]).

the pre-industrial era due to anthropogenic emissions of nitrogen oxides NO_x , and it continues to rise in many regions, driven by urbanization, industrial activity, and increasing temperatures.

Analogously to Rayleigh scattering, ozone absorption is described by an extinction coefficient k_{abs} defined as the product of the ozone number density $n_{\text{O}_3}(h)$ and its absorption cross section σ_{O_3} :

$$k_{\text{abs}}(h) = \sigma_{\text{O}_3} n_{\text{O}_3}(h), \quad (2.28)$$

with an implicit dependence on wavelength.

2.3 Limb observation geometry

In limb-scattering measurements, the viewing geometry differs fundamentally from the nadir configuration. In nadir observations, the instrument is directed toward the Earth’s surface, whereas limb-viewing instruments observe the atmosphere along lines of sight (LOS) that are nearly tangent to the Earth’s surface, i.e. toward the atmospheric horizon.

It is well known that while plane-parallel RTMs are suitable for nadir observations, they are not appropriate for limb geometry [41]. In this configuration, the curvature of the Earth and of the atmosphere must be explicitly taken into account. Accurate radiative transfer modeling for limb-viewing measurements therefore requires a *spherical* representation of the atmosphere. Assuming that atmospheric

properties vary only with altitude and not horizontally, the model is said to be a *spherical one-dimensional (1D) model*.

The LOS of a limb-viewing instrument follows a quasi-tangential path through the atmosphere. A key concept in limb geometry is the *tangent altitude* h_T , defined as the minimum distance between the LOS and the Earth’s surface. The corresponding location along the LOS is referred to as the *tangent point* **T** (see Figure 2.6). In practice, the instrument scans the LOS over a range of tangent altitudes, thereby providing a vertical profile of the limb radiance. This observing strategy is conceptually similar to occultation techniques, although in the case of limb scattering the LOS is not directed toward a light source such as the Sun.

The geometry of a limb-scattering measurement is illustrated in Figure 2.6. In an optically thin atmosphere, the sensitivity of the measured radiance to the atmospheric state is maximized near the tangent altitude. This is a direct consequence of the viewing geometry: the path length of the LOS is largest in the vicinity of the tangent altitude, leading to an enhanced contribution of this region to the measured signal [28]. For this reason, the tangent point is commonly used as a reference point to parameterize the measurement geometry in RTM codes such as SASKTRAN [29], Siro [26], and Gauss–Seidel limb scattering (GSLs) [42].

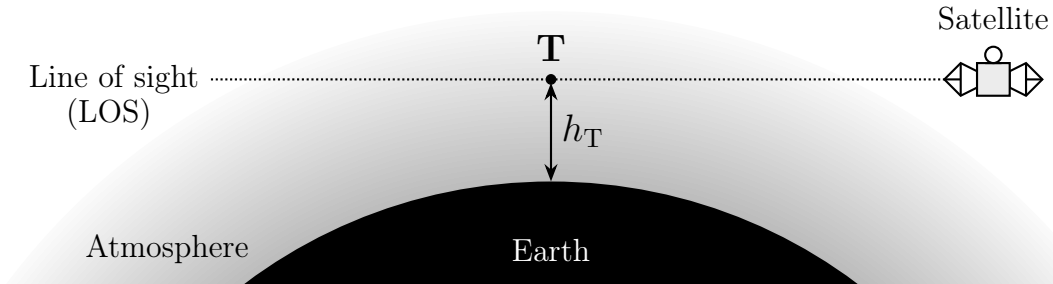


Figure 2.6: Geometry of a limb-scattering observation. The satellite observes the atmosphere along a LOS that is nearly tangent to the Earth’s surface. The minimum distance between the LOS and the surface defines the tangent altitude h_T , and the corresponding location is the tangent point **T** (adapted from Figure 2 in [29]).

In the present work, however, a different convention is adopted. Rather than defining the geometry with respect to the tangent point, the LOS and the associated viewing and illumination angles are defined at the location of the observer (i.e. the satellite). This choice provides a natural and consistent set of input parameters (summarized in Section 2.6) for the RTM. The information regarding the tangent point then becomes a derived quantity, determined by the viewing geometry (see Subsection 3.1).

2.4 Single-scattering approximation

In limb-scattering geometry, the instrument is located outside the atmosphere and observes radiation that originates from solar photons scattered into the instrument LOS. Photons emitted by the Sun may undergo one or several scattering events before reaching the detector. In the most general case, radiation reaching the in-

strument results from *multiple scattering processes*, including contributions from different atmospheric layers and, potentially, from the Earth's surface.

The full treatment of multiple scattering significantly complicates the solution of the radiative transfer equation (2.12), as the radiance at any point depends on contributions from all directions and from all previous scattering events. However, under certain conditions, a simplifying assumption can be introduced in order to find an analytical solution. In the middle atmosphere, where the number density of scattering particles is low, the probability that a photon undergoes multiple scattering events before reaching the detector becomes small. Although the optical path along the LOS may be long in limb geometry, the medium can be considered optically thin, meaning that the optical thickness associated with scattering processes remains sufficiently small for higher-order scattering contributions to be negligible.

This motivates the use of the *single-scattering approximation*, in which it is assumed that photons contributing to the measured radiance are scattered only once in the atmosphere and have not undergone any prior scattering before reaching the detector. Photons that have been scattered more than once, or that were scattered by the ground before reaching the detector, are classified as multiply scattered and are neglected. An illustration of single and multiple scattering contributions is shown in Figure 2.7, highlighting the different scattering paths of the solar beam into the instrument LOS.

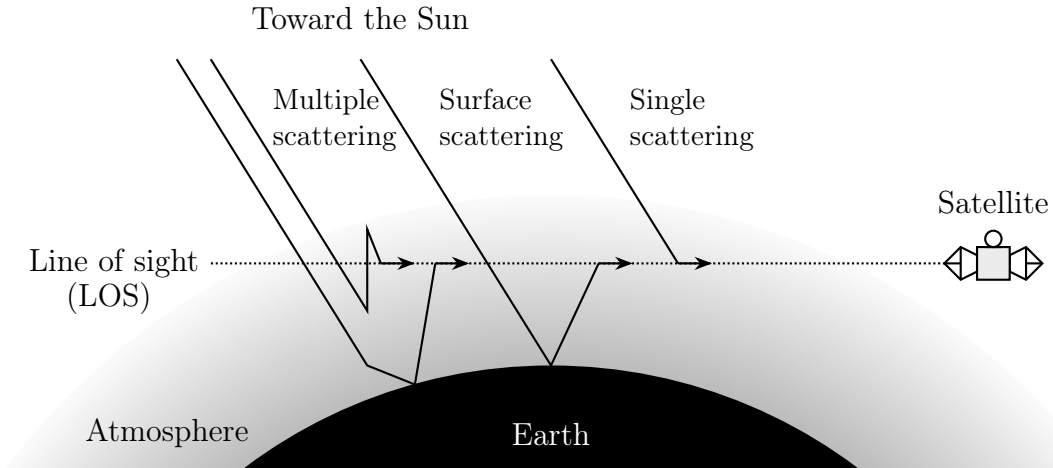


Figure 2.7: Schematic representation of the limb-viewing geometry. Photon paths involving single, surface, and multiple scattering contribute to the radiance measured along the LOS (adapted from Figure 1 in [29]).

The integral form of the radiative transfer equation (2.16) can be rewritten in terms of the observer position $\vec{r}_0$ and the propagation direction $\hat{\Omega}$ ⁵ [43],

$$I(\vec{r}_0, \hat{\Omega}) = I_{\text{end}}(s_{\text{end}}, \hat{\Omega})e^{-\tau(s_{\text{end}}, 0)} + \int_{s_{\text{end}}}^0 k(s)J(s, \hat{\Omega})e^{-\tau(s, 0)}ds, \quad (2.29)$$

where the path endpoint s_{end} corresponds to the top of the atmosphere in limb-viewing geometry, since the LOS does not intersect the Earth's surface.

The boundary term $I_{\text{end}}(s_{\text{end}}, \hat{\Omega})$ represents incoming radiation at the top of the atmosphere along the LOS. In limb geometry, this direction points toward space,

⁵The path length coordinate s is still used for terms that are evaluated along the LOS.

where no significant radiation source is present. Consequently, this term is assumed to be zero, except in the special case where the observation direction $-\hat{\Omega}$ is directly towards the Sun, which is excluded here [29].

Under the single-scattering approximation, only the *single scatter source term* $J_1(s, \hat{\Omega})$ is retained, and the radiance reduces to

$$I(\vec{r}_0, \hat{\Omega}) = \int_{s_{\text{end}}}^0 k(s) J_1(s, \hat{\Omega}) e^{-\tau(s,0)} ds. \quad (2.30)$$

The single scatter source term $J_1(s, \hat{\Omega})$ is obtained by considering the attenuation of the solar beam to each point s along the LOS, followed by scattering into the propagation direction $\hat{\Omega}$:

$$J_1(s, \hat{\Omega}) = \frac{k_{\text{scatt}}(s)}{k(s)} \frac{1}{4\pi} F(\hat{\Omega}_{\odot}) e^{-\tau(\text{Sun},s)} p(s, \Theta), \quad (2.31)$$

where $F(\hat{\Omega}_{\odot})$ is the incident solar spectral irradiance, $\tau(\text{Sun}, s)$ is the optical thickness along the solar path to the scattering point, and $p(s, \Theta)$ is the scattering phase function. The scattering angle Θ is defined as the angle between the incident solar direction $\hat{\Omega}_{\odot}$ and the observation direction $\hat{\Omega}$, such that

$$\cos \Theta = \hat{\Omega} \cdot \hat{\Omega}_{\odot}. \quad (2.32)$$

Since the solar beam is the only source of light for the first order scattering, the integral over all incoming directions in the general source term (2.13) simplifies to Equation (2.31), as the solar direction is a delta function in solid angle.

The single-scattered radiance (2.30) can be evaluated through direct numerical integration and is therefore a commonly used approximation for the scattered radiance in limb-scattering applications.

2.5 Geometric framework and coordinate systems

As with any physical modeling problem, the definition of appropriate reference frames and coordinate systems is essential. In the context of radiative transfer modeling, the position of the observer and the propagation geometry must be clearly defined. This section introduces the geometric concepts, reference systems, and coordinate transformations that are used throughout this work.

2.5.1 Reference ellipsoid and World Geodetic System 1984

As a first approximation, the Earth may be considered as a perfect sphere of mean radius $R_E = 6371$ km. However, due to its rotation about its axis, as theorized by Sir Isaac Newton and Christiaan Huygens in the 17th century, the Earth is slightly flattened at the poles and bulged at the equator.

In geodesy, a more accurate representation of the Earth's shape is therefore achieved using a reference ellipsoid. A *reference ellipsoid* is a mathematical surface of revolution obtained by rotating an ellipse about its minor axis. An ellipse is characterized by its *semi-major* and *semi-minor axes*, denoted a and b , respectively.

Table 2.1: The four WGS 84 defining parameters and two derived geometric constants (from [44]).

Parameters	Notations	Values
Earth’s semi-major axis	a	6 378 137.0 m
Earth’s flattening	f	1/298.257 223 563
Earth’s nominal mean angular velocity	ω	$7.292\,115 \times 10^{-5} \text{ rad s}^{-1}$
Geocentric gravitational constant	GM_E	$3.986\,004\,418 \times 10^{14} \text{ m}^3 \text{ s}^{-2}$
Earth’s semi-minor axis	b	6 356 752.3 m
Earth’s first eccentricity	e	0.081 819

From these two parameters, the *squared first eccentricity* e^2 and the *flattening* f are defined as

$$e^2 = \frac{a^2 - b^2}{a^2} = 1 - \frac{b^2}{a^2}, \quad (2.33)$$

$$f = \frac{a - b}{a} = 1 - \frac{b}{a}. \quad (2.34)$$

Since an ellipsoid is a surface obtained by rotating an ellipse around its minor axis, an ellipsoid can be fully defined by specifying any pair of parameters of the generating ellipse, except for (e^2, f) , since these are related by

$$e^2 = 2f - f^2. \quad (2.35)$$

Historically, the parameters of the Earth’s ellipsoid (the equatorial radius, the polar radius, and the flattening) were determined from arc measurements. Numerous reference ellipsoids have been proposed and used to model the Earth on a local or global scale. Since the second half of the 20th century, these methods have been replaced by global geodetic networks and satellite geodesy, allowing for highly precise determination of Earth’s geometric parameters.

The reference ellipsoid adopted here is the *World Geodetic System 1984* (WGS 84) *ellipsoid*, widely used in cartography and satellite navigation systems such as Global Positioning System (GPS). It is defined by four fundamental parameters: the semi-major axis a of the WGS 84 ellipsoid, the Earth’s flattening f , the Earth’s nominal mean angular velocity ω , and the geocentric gravitational constant GM_E , that is, the product of the Newtonian constant of gravitation $G = 6.674\,30 \times 10^{-11} \text{ m}^3 \text{ kg}^{-1} \text{ s}^{-2}$ and the mass of the Earth $M_E = 5.972\,186\,4 \times 10^{24} \text{ kg}$. The pair (a, f) fully defines the geometry of the ellipsoid, while (ω, GM_E) determine the associated normal gravity field. The values of these parameters (as well as derived parameters) are listed in Table 2.1.

An ellipsoidal model describes the Earth’s geometry and its associated normal gravity field. In practice, such a model is embedded within a geodetic datum. A *geodetic datum* is a coherent set of parameters and conventions defining a terrestrial reference frame, enabling positions on Earth to be expressed precisely. It specifies the reference ellipsoid, the origin, the orientation of the axes, and the scale of the coordinate system.

WGS 84 defines an *Earth-centered, Earth-fixed* (ECEF) *geocentric terrestrial reference system* and a global geodetic datum. The WGS 84 coordinate system is a right-handed Cartesian coordinate system shown in the Figure 2.9 and defined as follows:

- The coordinate origin $\mathbf{O}$, that is, the center of the WGS 84 ellipsoid, is located at the Earth's center of mass;
- The $\hat{z}$ -axis points toward the International Reference Pole, which does not exactly coincide with the Earth's rotational axis;
- The $\hat{x}$ -axis lies in the equatorial plane and passes through the intersection with the International Reference Meridian, which corresponds to the prime meridian and differs slightly from the Greenwich meridian;
- The $\hat{y}$ -axis completes the right-handed orthogonal system.

Any position vector $\vec{r}$ can therefore be expressed in ECEF coordinates as

$$\vec{r} = x\hat{x} + y\hat{y} + z\hat{z} \equiv (x, y, z). \quad (2.36)$$

Points located on the surface of the ellipsoid satisfy the Cartesian equation

$$\frac{x^2 + y^2}{a^2} + \frac{z^2}{b^2} = 1. \quad (2.37)$$

The WGS 84 reference frame has undergone several refinements since its initial realization in 1987. Each realization is defined by a set of control points at a specific epoch, reflecting time-dependent movements on the Earth's surface, such as plate tectonics. The current realization, designated as WGS 84 (G2296), is aligned at the centimeter level with the International Terrestrial Reference Frame 2020 (ITRF 2020), which provides the global geodetic reference for high-precision positioning.

2.5.2 Geodetic coordinates

Geodetic coordinates form a curvilinear coordinate system based on the reference ellipsoid. A point is described by its geodetic latitude φ , longitude λ , and ellipsoidal height h . *Geodetic latitude* φ is defined as the angle between the equatorial plane, defining 0° latitude, and the normal to the ellipsoid $\hat{n}$ at the point of interest. It ranges from -90° to 90° . *Longitude* λ is the angle between the prime meridian, defining 0° longitude, and the meridian passing through the point. It is typically expressed in degrees ranging from -180° to $+180^\circ$, with positive values eastward. *Ellipsoidal height* h is the distance measured along the ellipsoid normal vector $\hat{n}$ between the point of interest and the reference ellipsoid surface⁶. It is a signed distance such that it is positive outside the ellipsoid and negative inside. These definitions are illustrated in Figure 2.8.

Within the WGS 84 datum, conversion from geodetic coordinates (φ, λ, h) to ECEF Cartesian coordinates (x, y, z) is given by

$$\begin{aligned} x &= (N(\varphi) + h) \cos \varphi \cos \lambda, \\ y &= (N(\varphi) + h) \cos \varphi \sin \lambda, \\ z &= ((1 - f)^2 N(\varphi) + h) \sin \varphi, \end{aligned} \quad (2.38)$$

⁶In the following, the terms *ellipsoidal height* and *altitude* are used interchangeably and refer to the geometric height above the WGS 84 reference ellipsoid.

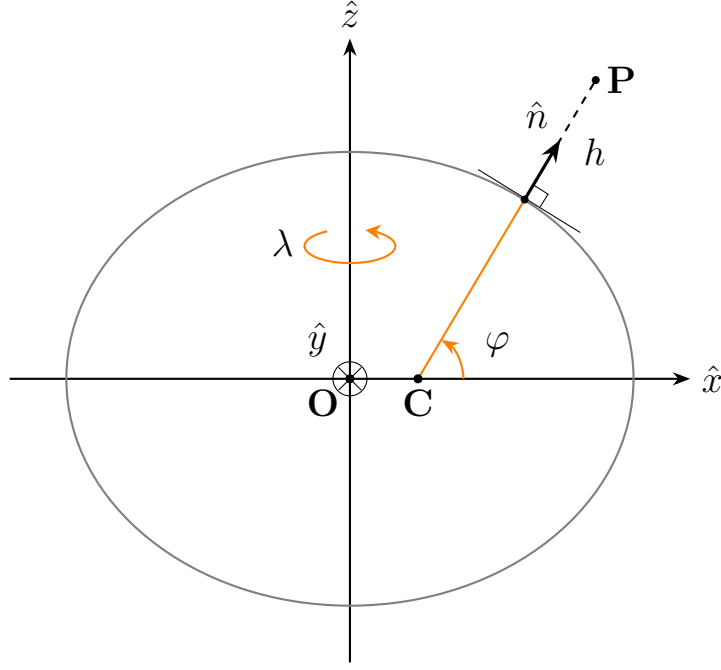


Figure 2.8: Definition of geodetic coordinates on a reference ellipsoid. A point $\mathbf{P}$ is located by its ellipsoidal height h measured along the ellipsoid normal vector $\hat{n}$. The geodetic latitude φ is defined as the angle between the equatorial plane and the normal $\hat{n}$. The longitude λ represents the rotation around the polar axis $\hat{z}$ from the prime meridian $\hat{x}$.

where

$$N(\varphi) = \frac{a}{\sqrt{1 - e^2 \sin^2 \varphi}} \quad (2.39)$$

is the prime vertical radius of curvature (defined in the Subsection 2.5.4).

The inverse transformation from ECEF to geodetic coordinates generally requires iterative numerical methods presented in [45].

2.5.3 Local reference frame : ENU coordinates

For many applications, it is convenient to define a local coordinate system attached to a specific point. The *local East-North-Up* (ENU) frame is a Cartesian system whose origin is located at a chosen point (on the Earth's surface, above or below it).

At any point on the ellipsoid, a tangent plane can be defined perpendicular to the ellipsoid normal. The ENU frame is constructed as follows:

- $\hat{E}$ points toward the east;
- $\hat{N}$ points toward the north;
- $\hat{U}$ points upward along the ellipsoidal normal.

The unit vectors of the ENU frame expressed in ECEF coordinates are given by

$$\begin{aligned} \hat{E} &= (-\sin \lambda, \cos \lambda, 0), \\ \hat{N} &= (-\cos \lambda \sin \varphi, -\sin \lambda \sin \varphi, \cos \varphi), \\ \hat{U} &= (\cos \lambda \cos \varphi, \sin \lambda \cos \varphi, \sin \varphi). \end{aligned} \quad (2.40)$$

Conversely, the ECEF basis vectors expressed in the ENU frame are

$$\begin{aligned}\hat{x} &= (-\sin \lambda, -\cos \lambda \sin \varphi, \cos \lambda \cos \varphi), \\ \hat{y} &= (\cos \lambda, -\sin \lambda \sin \varphi, \sin \lambda \cos \varphi), \\ \hat{z} &= (0, \cos \varphi, \sin \varphi).\end{aligned}\tag{2.41}$$

The relationship between the global ECEF frame and the local ENU frame is illustrated in Figure 2.9.

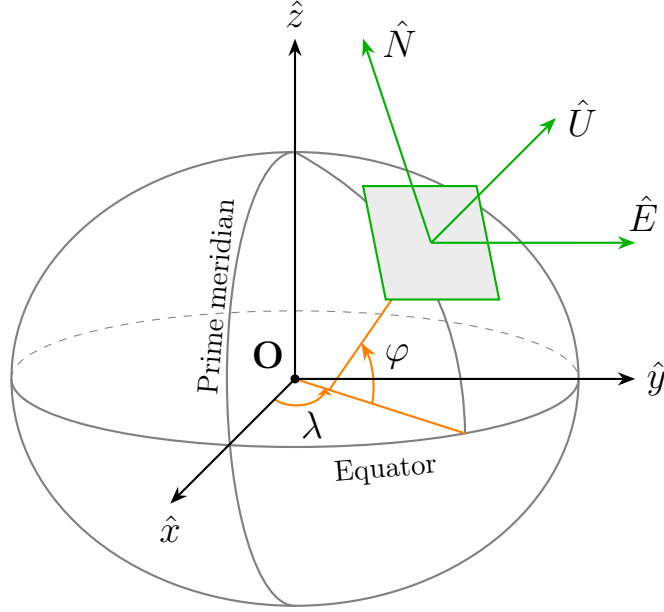


Figure 2.9: Representation of the ECEF and local ENU coordinate systems. The global frame $(\hat{x}, \hat{y}, \hat{z})$ is centered at the origin $\mathbf{O}$, while the tangent plane at a certain point on the ellipsoid, at geodetic latitude φ and longitude λ , supports the local frame $(\hat{E}, \hat{N}, \hat{U})$, corresponding to the East, North, and Up directions. The equator and the prime meridian are shown for reference.

Just as in astronomy, a local horizontal coordinate system can be defined using the ENU frame. Given a unit direction vector $\hat{u}$ expressed in ENU coordinates, the elevation angle ϵ and azimuth angle ϕ are defined as

$$\epsilon = \arcsin(\hat{u} \cdot \hat{U}),\tag{2.42}$$

$$\phi = \text{atan2}(\hat{u} \cdot \hat{E}, \hat{u} \cdot \hat{N}).\tag{2.43}$$

The *elevation angle* ϵ ranges from -90° to 90° , while the *azimuth angle* ϕ is typically defined in the interval $[0^\circ, 360^\circ]$, measured clockwise from north.

Hence, the components of the unit vector $\hat{u}$ can be expressed as

$$\begin{aligned}\hat{u} \cdot \hat{E} &= \cos \epsilon \sin \phi, \\ \hat{u} \cdot \hat{N} &= \cos \epsilon \cos \phi, \\ \hat{u} \cdot \hat{U} &= \sin \epsilon.\end{aligned}\tag{2.44}$$

An alternative quantity frequently used is the *zenith angle* θ , defined as the complement of the elevation angle:

$$\theta = 90^\circ - \epsilon.\tag{2.45}$$

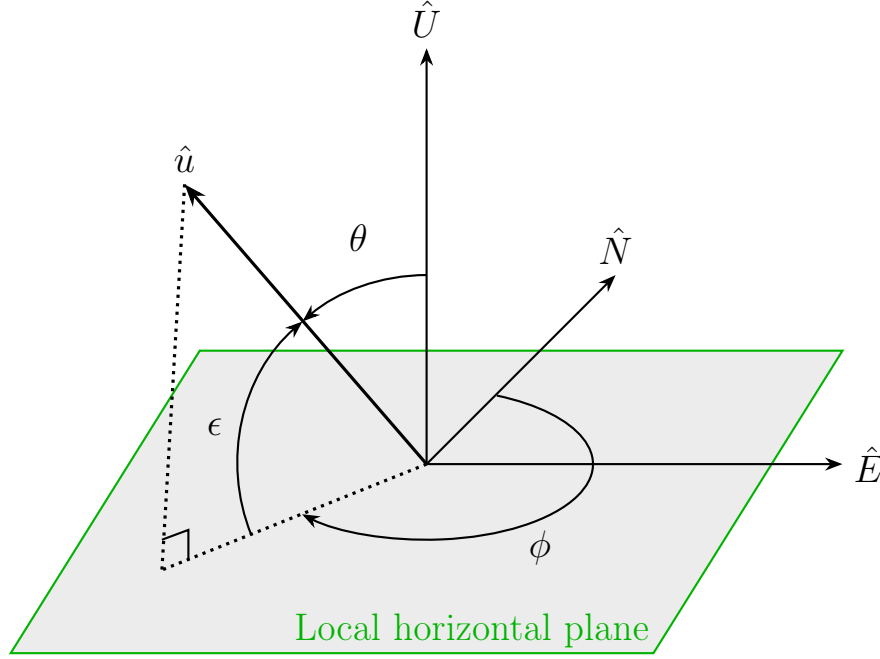


Figure 2.10: Definition of the angles associated with a unit direction vector $\hat{u}$ in the local ENU frame. The azimuth angle ϕ is defined in the horizontal plane as the angle measured clockwise from north $\hat{N}$ to the projection of $\hat{u}$. The zenith angle θ is defined as the angle between $\hat{u}$ and the vertical direction $\hat{U}$. The elevation angle ϵ is measured between $\hat{u}$ and the horizontal plane, such that $\epsilon = 90^\circ - \theta$.

These angles are illustrated in Figure 2.10.

In particular, these definitions are useful for describing illumination conditions. At any point in space, the position of the Sun can be specified by the *solar zenith angle* $\theta_\odot$ and the *solar azimuth angle* $\phi_\odot$.

2.5.4 Osculating sphere

Although representing the Earth as an ellipsoid of revolution significantly reduces the errors associated with a purely spherical approximation, some considerations arise when modeling radiative transfer through the atmosphere. In particular, the computation of photon paths requires an accurate description of the local geometry encountered by radiation propagating toward the detector. For this reason, it is useful to associate a locally equivalent sphere with each point. This sphere's center generally does not coincide with the ellipsoid center $\mathbf{O}$, but rather with a point $\mathbf{C}$ (as illustrated in Figure 2.8), and its radius depends on the point location and the direction of measurement from that point.

This construction corresponds to the *osculating sphere*, defined as the best local spherical approximation to the ellipsoid in the vicinity of a given point. Its radius can be directly estimated from the curvature of the Earth at the point of interest. A proper definition of this concept requires elements of differential geometry presented, e.g., in [45, 46].

Consider a curve lying on the ellipsoid surface, such as a meridian arc or a parallel. The *curvature* κ of this curve quantifies the rate at which its tangent direction changes along the curve. For a surface, however, curvature naturally depends on

the direction in which the surface is traversed.

Curvature can be rigorously defined through normal sections. A *normal section* of a surface at a given point is the curve obtained by the intersection of that surface with a plane containing the surface normal at that point, called a *normal plane*. Among all possible normal sections, two directions are of particular importance: those corresponding to the maximum and minimum curvature. These define the *principal curvatures*, and the directions of their corresponding tangent vectors are orthogonal and referred to as the *principal normal directions*. The reciprocal of the curvature defines the *radius of curvature* $R = 1/\kappa$ and the radii associated with the principal curvatures are called the *principal radii of curvature*.

In the case of the Earth's ellipsoid, the curvature is maximal in the north-south direction and minimal in the perpendicular east-west direction. The two principal normal sections are therefore: the *meridian normal section*, aligned with the local meridian and the *prime vertical normal section*, perpendicular to the meridian. The corresponding principal radii of curvature at a point of geodetic latitude φ are given by

$$M(\varphi) = \frac{a(1 - e^2)}{(1 - e^2 \sin^2 \varphi)^{3/2}}, \quad (2.46)$$

for the *Earth's meridional radius of curvature*, and

$$N(\varphi) = \frac{a}{\sqrt{1 - e^2 \sin^2 \varphi}}, \quad (2.47)$$

for the *Earth's prime vertical radius of curvature*.

At any point on the ellipsoid, M and N represent respectively the minimum and maximum radii of curvature among all normal sections. It follows directly that $M \leq N$ for all φ , with equality occurring at the poles, that is, $\varphi = \pm 90^\circ$.

To determine the radius of curvature along an arbitrary direction, the orientation of the normal section is required. This is done using the *normal section azimuth* α , defined as the angle measured clockwise from the north direction within the tangent plane to the ellipsoid at the point of interest (distinct from the previously defined azimuth angle ϕ).

Euler's formula from differential geometry gives the curvature κ_α of a normal section oriented at azimuth α in terms of the principal radii of curvature:

$$\kappa_\alpha = \frac{1}{R_\alpha} = \frac{\sin^2 \alpha}{N} + \frac{\cos^2 \alpha}{M}. \quad (2.48)$$

The corresponding radius R_α defines the radius of the osculating sphere associated with that specific direction.

The center of this osculating sphere coincides with the *center of curvature* at the considered point on the ellipsoid and is generally offset from the center of the ellipsoid. For a point with ECEF coordinates (x, y, z) on the surface, the coordinates of the center $\mathbf{C}_\alpha$ of the osculating sphere of radius R_α can be expressed as

$$\mathbf{C}_\alpha = (x, y, z) - R_\alpha \hat{n}, \quad (2.49)$$

where $\hat{n}$ denotes the outward normal vector to the ellipsoid at that point.

2.6 Summary and assumptions

This section summarizes the RTM developed throughout this chapter, including the expression of the single-scattered radiance, the required model inputs, and the underlying physical assumptions. It thus serves as a bridge to the next chapter, which focuses on the practical and numerical implementation of this RTM.

2.6.1 Single-scattered radiance formulation

By combining Equations (2.30) and (2.31), the radiance observed at position $\vec{r}_0$ in direction $\hat{\Omega}$ due to a single scattering event of solar photons can be expressed as a line integral along the LOS:

$$I(\vec{r}_0, \hat{\Omega}) = F(\hat{\Omega}_{\odot}) \int_{s_{\text{end}}}^0 e^{-\tau(\text{Sun}, s)} k_{\text{scatt}}(s) \bar{p}(s, \Theta) e^{-\tau(s, 0)} ds, \quad (2.50)$$

where the *effective phase function* is defined as

$$\bar{p}(s, \Theta) = \frac{p(s, \Theta)}{4\pi}. \quad (2.51)$$

The single-scattered radiance is obtained by integrating contributions from all scattering points along the LOS. As illustrated in Figure 2.11, each contribution is weighted by three processes: (i) attenuation of the solar beam to the scattering point, $e^{-\tau(\text{Sun}, s)}$; (ii) local scattering and angular redistribution into the LOS through $k_{\text{scatt}}(s) \bar{p}(s, \Theta)$; and (iii) attenuation of the scattered radiation toward the observer, $e^{-\tau(s, 0)}$.

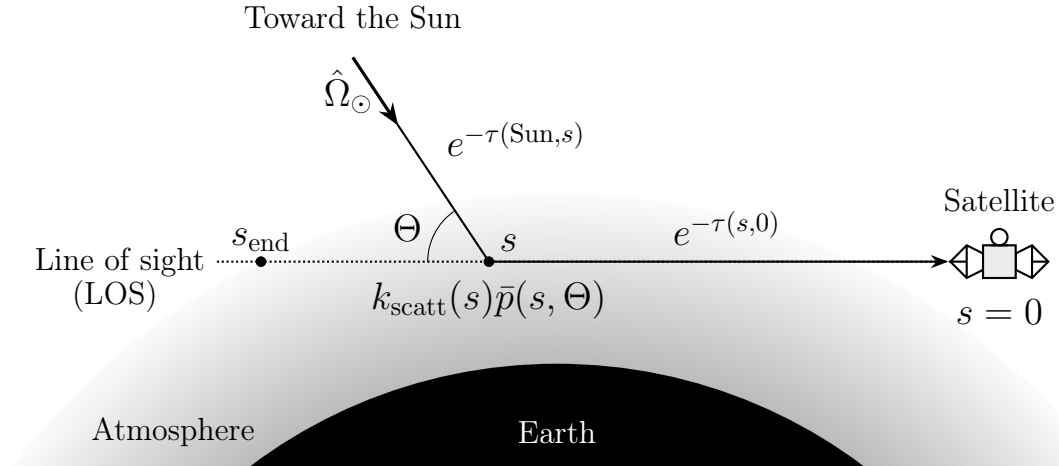


Figure 2.11: Schematic representation of the single-scattering contribution to the radiance along the LOS. Solar photons, propagating in the direction $\hat{\Omega}_{\odot}$, are attenuated along their path to a scattering point s through $e^{-\tau(\text{Sun}, s)}$, scattered locally according to the scattering coefficient and effective phase function $k_{\text{scatt}}(s) \bar{p}(s, \Theta)$, and further attenuated along the LOS toward the observer through $e^{-\tau(s, 0)}$. The total radiance results from the integration of these contributions over all scattering points s between s_{end} and $s = 0$.

2.6.2 Model inputs and outputs

For a given wavelength, the computation of the radiance along a LOS requires the following inputs:

- The satellite position, specified either in geodetic coordinates $(\varphi_0, \lambda_0, h_0)$ or in ECEF Cartesian coordinates $\vec{r}_0 = (x_0, y_0, z_0)^T$;
- The solar direction at the satellite position, given by the solar zenith and azimuth angles $(\theta_\odot^0, \phi_\odot^0)$;
- The LOS azimuth angle α_{LOS}^0 in the local tangent plane at the satellite position;
- The desired tangent altitude h_T ;
- The atmospheric state, described by altitude-dependent air number density $n_{\text{air}}(h)$ and ozone number density $n_{\text{O}_3}(h)$.

In practice, the instrument samples multiple LOS corresponding to different tangent altitudes, thereby producing a vertical radiance profile. Since the radiance is obtained through direct line integration, the computational cost remains relatively low and depends only on the number of LOS [47].

2.6.3 Model assumptions and justification

The RTM developed in this work relies on several simplifying assumptions, which are summarized and justified below.

Single-scattering approximation The most critical assumption is that only single-scattering events contribute to the measured radiance, while multiple scattering is neglected. This approximation is valid in optically thin conditions, particularly in the middle atmosphere where particle densities are low. At short UV wavelengths (below 300 nm), strong ozone absorption significantly attenuates photons, reducing the probability of multiple scattering. In this regime, the limb radiance is well represented by single scattering alone [48]. At longer wavelengths, however, the contribution of multiple scattering increases and can represent a substantial fraction of the total signal. Nevertheless, even in such cases, the dominant contributions often arise from first- and second-order scattering [29]. More advanced RTMs account for multiple scattering using numerical techniques such as the method of successive orders of scattering [29] or Monte Carlo simulations [26, 43]. These approaches iteratively build higher-order scattering contributions or statistically estimate photon trajectories, at the cost of increased computational complexity. The validity of the single-scattering approximation adopted in this work will be assessed through comparisons with simulations performed using the SASKTRAN model in Subsection 3.6.5.

Neglect of refraction Photon paths are assumed to be straight lines, neglecting atmospheric refraction. This approximation is justified because refractive bending is generally small at the altitudes relevant for limb-scattering observations. Consequently, the associated error remains limited for the applications considered here.

⁷The index 0 is used consistently to denote quantities defined at the observer/satellite location.

Spherical symmetry (1D atmosphere) The atmosphere is assumed to be spherically symmetric, with all physical properties depending only on altitude h . This reduces the problem to a 1D spherical model. More advanced RTMs may account for horizontal variations in atmospheric properties and are therefore fully three-dimensional (3D). Intermediate approaches, such as *pseudo-spherical models*, retain spherical geometry for photon paths while approximating the atmosphere as plane-parallel in the radiative transfer calculation [27]. The 1D spherical assumption adopted here provides a good compromise between physical realism and computational efficiency.

Neglect of polarization (scalar approximation) The model uses a scalar radiative transfer formulation, neglecting polarization effects. In the full vector formulation, scattering is described by 4×4 phase matrices acting on the four-element Stokes vector, which contains both radiance and polarization information. However, for single scattering of unpolarized solar radiation, the scalar and vector intensities are equivalent. Therefore, neglecting polarization does not introduce errors in the single-scattered radiance itself [48].

Rayleigh scattering and ozone absorption only Only Rayleigh scattering and ozone absorption are included in the model. Other processes, such as aerosol (Mie) scattering and absorption by additional atmospheric constituents, are neglected. This assumption is justified in the short spectral range ($\lambda < 400$ nm) and at higher altitudes. Above approximately 40 km, aerosol concentrations are generally very low, such that their contribution to the extinction and scattering becomes negligible compared with molecular (Rayleigh) scattering. Moreover, at the shortest wavelengths, the limb radiance is essentially insensitive to stratospheric aerosols. At longer wavelengths, aerosol scattering can enhance the radiance at higher altitudes while increasing extinction at lower altitudes [31].

Overall, the RTM presented here is a 1D *spherical scalar model* based on the single-scattering approximation. Despite these simplifications, the model captures the dominant physical processes governing limb-scattered radiance in the middle atmosphere.

Chapter 3

Numerical implementation of the radiative transfer model

The previous chapter introduced the theoretical framework of the single-scattering RTM and the physical assumptions used throughout this work. The present chapter focuses on the numerical implementation of this model and describes the complete computational pipeline leading from the user-defined inputs to the calculated limb-scattered radiance. The RTM was entirely implemented in Python.

3.1 Viewing geometry

The construction of the viewing geometry constitutes the first step of the radiative transfer calculation. Since limb-scattering observations are highly sensitive to the tangent altitude and to the LOS orientation, the determination of the tangent point coordinates together with the LOS direction therefore plays a central role in the overall radiative transfer calculation.

The user first specifies the satellite position in geodetic coordinates $(\varphi_0, \lambda_0, h_0)$. Although geodetic coordinates remain useful for user inputs and for the interpretation of the results, most geometric calculations are performed in the ECEF frame. In particular, propagation directions, LOS vectors, and positions are all computed in Cartesian coordinates. Consequently, the satellite coordinates are converted into ECEF coordinates using the **Transformer** module of the Python library **pyproj**, which relies internally on the PROJ coordinate transformation software [49]. The EPSG:4979 coordinate system is used for geodetic coordinates whereas EPSG:4978 is used for ECEF Cartesian coordinates.

The first geometric quantities required by the model are the *viewing direction*

$$\hat{u} = -\hat{\Omega}, \quad (3.1)$$

also referred to in the following as the *LOS unit vector*, pointing from the satellite towards the atmosphere, and the tangent point **T**.

These two quantities are intrinsically coupled. For a given LOS, the tangent point can be determined geometrically. However, in this case, the user specifies a desired tangent altitude h_T together with the LOS azimuth angle α_{LOS}^0 at the satellite position. The model must therefore iteratively determine the viewing direction producing the required tangent altitude.

The viewing geometry calculation is consequently divided into two successive problems:

1. Determining the tangent point associated with a known LOS;
2. Determining the LOS unit vector corresponding to a prescribed tangent altitude.

3.1.1 Determination of the tangent point

Consider a satellite located at position $\vec{r}_0$ in ECEF coordinates and a LOS unit vector $\hat{u}$. The LOS may be parameterized by the path coordinate s as

$$\vec{r}(s) = \vec{r}_0 + \hat{u}s. \quad (3.2)$$

The tangent point corresponds to the point of minimum altitude along this LOS. In other words, there exists a path coordinate s_T such that the tangent point position is given by

$$\vec{r}_T = \vec{r}_0 + \hat{u}s_T. \quad (3.3)$$

Spherical Earth geometry

Finding the point on a line that is closest to the surface of an ellipsoidal Earth model such as WGS 84 is not straightforward. However, for a perfectly spherical Earth, this problem admits a simple analytical solution.

In the spherical case, the tangent point is simply the point on the LOS closest to the Earth's center. Determining the tangent point therefore reduces to minimizing the distance between the propagation ray and the origin. The optimization problem may therefore be formulated by minimizing the loss function

$$\frac{1}{2} \|\vec{r}_0 + \hat{u}s\|^2. \quad (3.4)$$

The tangent path coordinate satisfies

$$s_T = \arg \min_s \frac{1}{2} \|\vec{r}_0 + \hat{u}s\|^2 \iff \left. \frac{d \left(\frac{1}{2} \|\vec{r}_0 + \hat{u}s\|^2 \right)}{ds} \right|_{s_T} = 0. \quad (3.5)$$

Differentiation with respect to s immediately gives

$$s_T = -\vec{r}_0 \cdot \hat{u}. \quad (3.6)$$

This spherical approximation is used only to construct an initial estimate for the more general ellipsoidal problem.

Ellipsoidal Earth geometry

Unlike the spherical case, the point of minimum altitude along a ray is not equivalent to the point closest to the Earth's center. The tangent point must instead be defined relative to the ellipsoidal surface.

For a given LOS, the problem consists in finding the point $\mathbf{S}$ located on the ellipsoid surface, with position vector

$$\vec{r}_S = (x_S, y_S, z_S), \quad (3.7)$$

together with the path coordinate s_T , such that the distance between the LOS and the ellipsoid is minimal.

The tangent point is therefore obtained by solving the constrained minimization problem

$$\arg \min_{x_S, y_S, z_S, s_T} \frac{1}{2} \|\vec{r}_T - \vec{r}_S\|^2 = \arg \min_{x_S, y_S, z_S, s_T} \frac{1}{2} \|\vec{r}_0 + \hat{u}s_T - \vec{r}_S\|^2, \quad (3.8)$$

under the constraint that surface point $\mathbf{S}$ must satisfy

$$f(x_S, y_S, z_S) = \frac{x_S^2 + y_S^2}{a^2} + \frac{z_S^2}{b^2} - 1 = 0. \quad (3.9)$$

The problem is solved numerically using the method of Lagrange multipliers. Introducing a multiplier μ , the Lagrangian becomes

$$\mathcal{L}(x, y, z, s, \mu) = \frac{1}{2} \|\vec{r}_0 + \hat{u}s - \vec{r}\|^2 + \mu f(x, y, z). \quad (3.10)$$

Differentiation of the Lagrangian $\mathcal{L}$ with respect to the variables $(\vec{r}, s, \mu)$ leads to a system of three equations (one vector equation and two scalar equations):

$$\vec{r}_0 + \hat{u}s_T - \vec{r}_S + \mu \nabla f(x_S, y_S, z_S) = 0, \quad (3.11)$$

$$\hat{u} \cdot (\vec{r}_0 + \hat{u}s_T - \vec{r}_S) = 0, \quad (3.12)$$

$$f(x_S, y_S, z_S) = 0. \quad (3.13)$$

This nonlinear system is initialized using the analytical spherical solution and solved using the Levenberg–Marquardt algorithm from the open-source library SciPy [50].

The numerical solution finally returns the quantities required for the subsequent radiative transfer calculations, namely the ellipsoidal surface point $\mathbf{S}$ and most importantly the tangent path coordinate s_T . The ECEF coordinates of the tangent point are then obtained through (3.3). Whenever latitude and longitude information are required, the Cartesian coordinates of the tangent point may finally be converted back into geodetic coordinates.

3.1.2 Determination of the line of sight

The previous subsection described how the tangent point can be determined for a known LOS unit vector $\hat{u}$. In practice, however, the LOS is not directly specified by the user. Instead, the model takes as input the LOS azimuth angle α_{LOS}^0 at the satellite position together with the desired tangent altitude h_T . The objective of this second step is therefore to determine the LOS unit vector producing the required tangent altitude.

The LOS direction is defined in the local ENU basis at the satellite position. Using the local basis vectors $(\hat{E}_0, \hat{N}_0, \hat{U}_0)$, expressed in ECEF coordinates through Equation (2.41), the LOS unit vector may be written as

$$\hat{u} = \cos \alpha_{\text{LOS}}^0 \cos \epsilon_{\text{LOS}}^0 \hat{N}_0 + \sin \alpha_{\text{LOS}}^0 \cos \epsilon_{\text{LOS}}^0 \hat{E}_0 + \sin \epsilon_{\text{LOS}}^0 \hat{U}_0, \quad (3.14)$$

where ϵ_{LOS}^0 denotes the elevation angle of the LOS at the satellite position.

The azimuth angle is directly prescribed by the user whereas the elevation angle remains unknown. The problem therefore consists in finding the elevation angle for which the resulting LOS produces the prescribed tangent altitude h_{T} .

As in the previous subsection, the spherical-Earth approximation provides a convenient analytical initial guess. For a perfectly spherical Earth of radius R_{E} , simple geometry leads to

$$\epsilon_{\text{LOS}}^0 = -\arccos\left(\frac{R_{\text{E}} + h_{\text{T}}}{R_{\text{E}} + h_0}\right), \quad (3.15)$$

where h_0 is the satellite altitude.

This spherical solution is used only as an initial estimate for the ellipsoidal case. A scalar function

$$g(\epsilon) = \text{alt}(\epsilon) - h_{\text{T}} \quad (3.16)$$

is then introduced, where $\text{alt}(\epsilon)$ denotes the tangent altitude obtained from the tangent-point algorithm described in the previous subsection for a LOS constructed with elevation angle ϵ .

The objective is therefore to determine the root of the equation

$$g(\epsilon_{\text{LOS}}^0) = 0. \quad (3.17)$$

This one-dimensional root-finding problem is solved numerically using the secant method [50]. At each iteration, a trial LOS is constructed from Equation (3.14), the associated tangent point is computed using the ellipsoidal tangent-point algorithm presented before, and the resulting tangent altitude is compared with the target value h_{T} .

Once convergence is achieved, the LOS unit vector is determined in ECEF coordinates by substituting the numerical solution ϵ_{LOS}^0 into Equation (3.14). This LOS vector is subsequently used throughout all radiative transfer calculations.

3.2 Osculating-sphere geometry

Once the tangent point and LOS have been determined, the local geometry required for the radiative transfer calculations can be constructed. In particular, the propagation geometry is locally approximated using an osculating sphere matching the curvature of the WGS 84 ellipsoid at the tangent point, as illustrated in Figure 3.1.

The first quantity required for this construction is the LOS azimuth angle at the tangent point, denoted $\alpha_{\text{LOS}}^{\text{T}}$. This angle is computed from Equation (2.43), where the vectors $\hat{E}$ and $\hat{N}$ now correspond to the local ENU basis defined at the tangent point.

Using the tangent-point latitude, the meridional and prime-vertical radii of curvature of the ellipsoid are then evaluated from Equations (2.46) and (2.47). Euler's curvature formula (2.48) subsequently gives the radius of curvature associated with the normal section oriented along the LOS azimuth direction $\alpha_{\text{LOS}}^{\text{T}}$:

$$R_{\alpha_{\text{LOS}}^{\text{T}}} = \left(\frac{\cos^2 \alpha_{\text{LOS}}^{\text{T}}}{M} + \frac{\sin^2 \alpha_{\text{LOS}}^{\text{T}}}{N} \right)^{-1}. \quad (3.18)$$

This is the radius of the osculating sphere, whose center is obtained by moving from the surface point $\mathbf{S}$ along the inward normal direction $-\hat{n}_S$ (see Figure 3.1). Using Equation (2.49), the ECEF coordinates of the center $\mathbf{C}_{\alpha_{\text{LOS}}^T}$ are therefore given by

$$\mathbf{C}_{\alpha_{\text{LOS}}^T} = \vec{r}_S - R_{\alpha_{\text{LOS}}^T} \hat{n}_S, \quad (3.19)$$

where the local outward normal vector $\hat{n}_S$ is obtained from the gradient of (3.9),

$$\nabla f(x_S, y_S, z_S) = 2 \left(\frac{x_S}{a^2}, \frac{y_S}{a^2}, \frac{z_S}{b^2} \right). \quad (3.20)$$

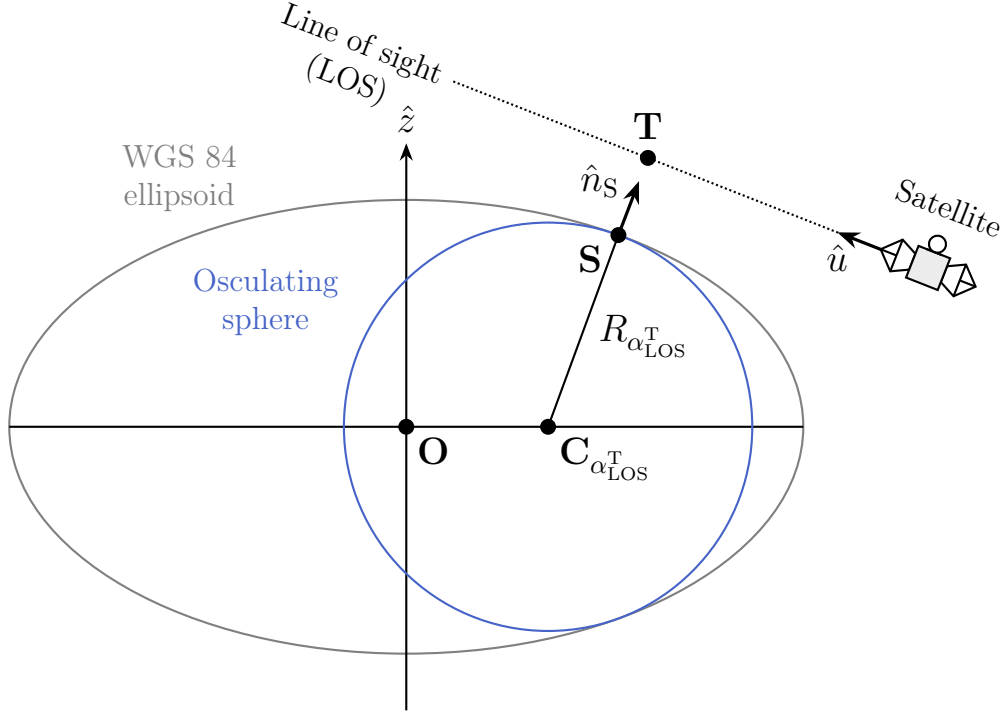


Figure 3.1: Geometry of the osculating-sphere construction at the tangent point $\mathbf{T}$. The WGS 84 ellipsoid is locally approximated by an osculating sphere whose radius equals the radius of curvature $R_{\alpha_{\text{LOS}}^T}$ associated with the LOS azimuth at the tangent point α_{LOS}^T . The center of the osculating sphere $\mathbf{C}_{\alpha_{\text{LOS}}^T}$ is obtained by moving from the surface point $\mathbf{S}$ along the inward normal direction $-\hat{n}_S$.

The resulting sphere constitutes a local spherical approximation of the ellipsoidal Earth preserving the local curvature encountered by the LOS near the tangent point. This considerably simplifies the subsequent geometric calculations involved in the RTM, including ray intersections with atmospheric layers.

By construction, the unit vector pointing from the center of the osculating sphere toward the tangent point coincides with the local zenith direction. Along this direction, a variation in the radial distance from the osculating-sphere center is exactly equal to a variation in altitude above the ellipsoidal surface. For directions other than the zenith, this is not exactly true.

3.3 Atmosphere

3.3.1 Atmospheric discretization

The local spherical geometry introduced in the previous section is used to discretize the atmosphere into *concentric spherical cells* above the Earth’s surface¹. In the present work, the atmosphere is divided into layers of 1 km thickness along the local zenith direction, extending from the surface up to an altitude of 100 km. The resulting *atmospheric grid* therefore consists of 100 individual layers.

In reality, the atmosphere does not terminate abruptly at an altitude of 100 km. Instead, atmospheric density decreases approximately exponentially with altitude as a consequence of hydrostatic equilibrium. In radiative transfer modeling, however, it is necessary to define a finite top-of-atmosphere altitude beyond which the atmosphere is neglected. Choosing a top-of-atmosphere altitude of 100 km introduces only negligible radiative errors compared to a full Chapman-layer representation [42].

Atmospheric quantities are defined at the center of each atmospheric layer, namely at altitudes of

$$0.5, 1.5, 2.5, \dots, 99.5 \text{ km.} \quad (3.21)$$

These mid-layer values define the atmospheric altitude grid used throughout the simulations. In the original implementation of SASKTRAN, atmospheric properties within each spherical cell were assumed to be homogeneous, independently of the position inside the layer. In the present implementation, however, atmospheric quantities are assumed to vary linearly with altitude between adjacent layer centers. This linear interpolation removes the artificial discontinuities and provides a more accurate representation of the atmosphere.

As discussed by Loughman et al. [42], assuming a linear variation of the extinction coefficient within atmospheric layers significantly improves the accuracy of single-scattering radiance calculations. In particular, they showed that assuming constant constituent concentrations within each layer can lead to underestimations of the single-scattered radiance of up to approximately 1% for tangent altitudes near 60 km. Implementing linear interpolation therefore constitutes an important improvement for high-altitude limb-scattering calculations.

3.3.2 Atmospheric parameters

All atmospheric parameters profiles used in the simulations are represented on the discretized altitude grid introduced previously. Consequently, each atmospheric quantity is described by a set of 100 values corresponding to the centers of the 100 atmospheric layers.

The atmosphere considered in this work is characterized by temperature and pressure profiles, denoted respectively by $T(h)$ and $P(h)$, obtained from reanalysis data of the atmosphere for the year 2017, produced by the Belgian Assimilation System for Chemical Observations (BASCOE) chemistry transport model [51]. The

¹Throughout this work, the term *spherical shell* refers to a spherical boundary surface separating two atmospheric layers, while the term *spherical cell* denotes the finite atmospheric layer bounded by two successive shells.

air number density profile $n_{\text{air}}(h)$ is then derived from the ideal gas law:

$$n_{\text{air}}(h) = \frac{P(h)}{k_{\text{B}} T(h)}. \quad (3.22)$$

The temperature and air number density profiles are presented in Figures 3.2 and 3.3, respectively. Furthermore, the Rayleigh scattering cross section as a function of wavelength is computed using the formulation described in Subsection 2.2.1.

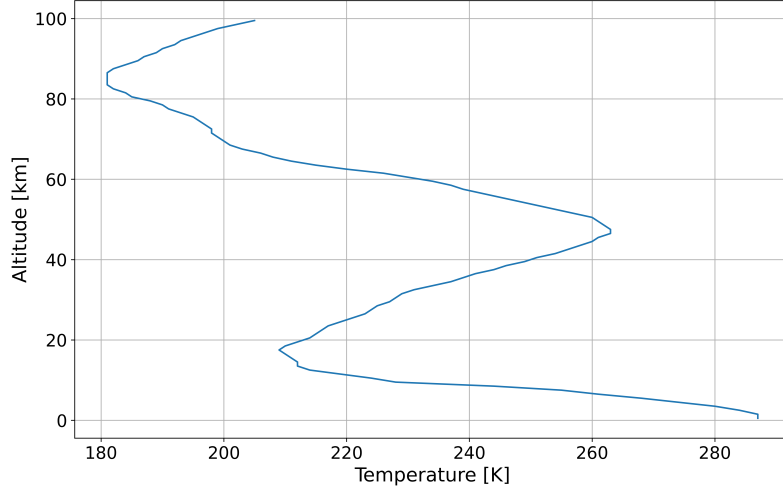


Figure 3.2: Temperature profile used in the radiative transfer simulations.

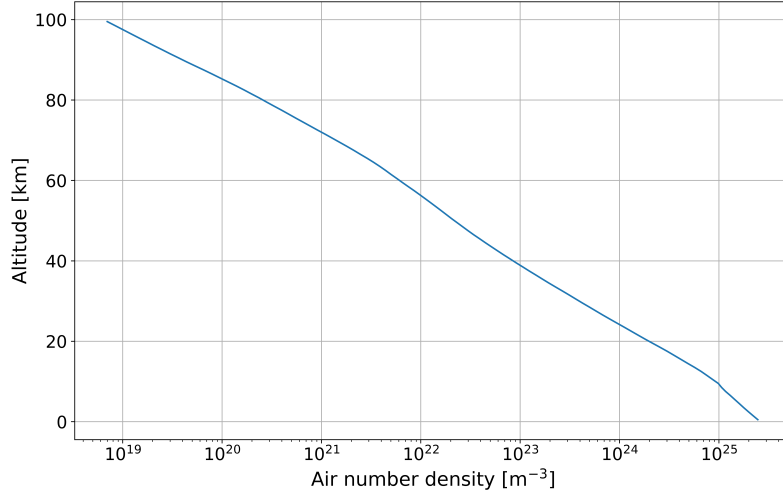


Figure 3.3: Air number density profile derived from the temperature and pressure profiles through the ideal gas law, shown on a logarithmic scale.

The second atmospheric constituent considered in this work is ozone. The ozone number density profile is also obtained from BASCOE model [51] and is shown in Figure 3.4. For the ozone absorption cross section, the measurements of Burrows et al. [38] are used in the spectral range extending from 231 nm to 794 nm at a temperature of 241 K. The corresponding spectrum is presented in Figure 3.5. Its overall structure is consistent with the reference spectrum shown in Figure 2.4. The remaining differences arise primarily from the temperature dependence of the

ozone absorption cross section. The temperature of 241 K was selected because it is representative of the typical temperatures encountered in the middle atmosphere.

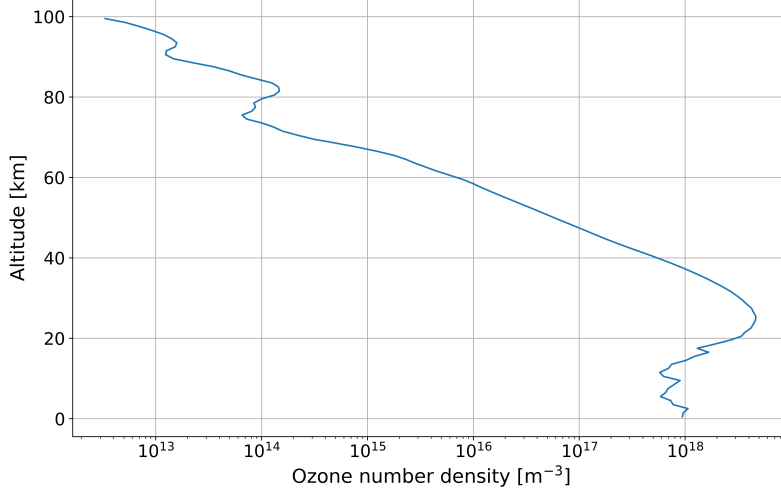


Figure 3.4: Ozone number density profile used in the radiative transfer simulations, shown on a logarithmic scale.

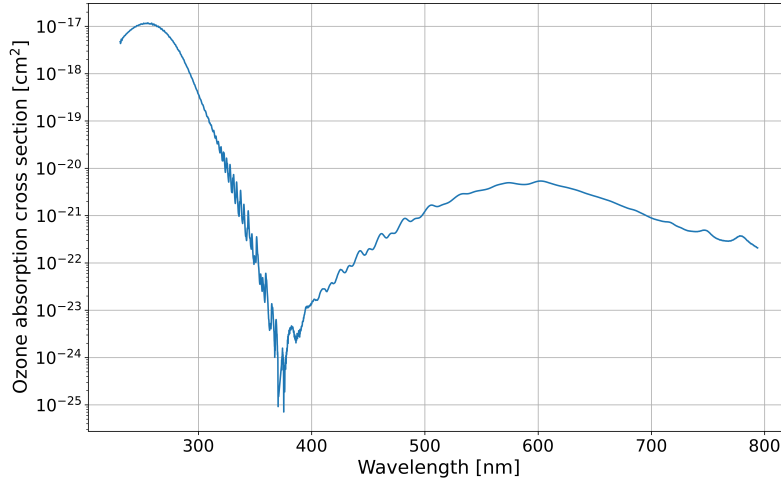


Figure 3.5: Ozone absorption cross section spectrum at 241 K in the 231–794 nm range, based on the measurements of Burrows et al. [38].

Using these atmospheric profiles and cross sections, the extinction coefficient associated with Rayleigh scattering $k_{\text{scatt}}(h)$ and the extinction coefficient associated with ozone absorption $k_{\text{abs}}(h)$ can be computed. The total extinction coefficient is then given by

$$k(h) = k_{\text{scatt}}(h) + k_{\text{abs}}(h). \quad (3.23)$$

The respective contributions of Rayleigh scattering and ozone absorption to the total extinction coefficient are shown for wavelengths of 310 nm, 350 nm, and 600 nm in Figures 3.6, 3.7, and 3.8. At 350 nm, ozone absorption is weak compared to Rayleigh scattering, such that the total extinction is dominated primarily by air scattering. In contrast, at 310 nm, ozone absorption becomes significant and dominates the total extinction in the altitude region corresponding to the ozone layer,

where ozone concentrations are largest. At 600 nm, the extinction profile exhibits a similar structure to that at 310 nm, although with magnitudes approximately one order of magnitude smaller. This reduction originates both from the weaker ozone absorption cross section at longer wavelengths and from the strong wavelength dependence of Rayleigh scattering, whose cross section scales as λ^{-4} .

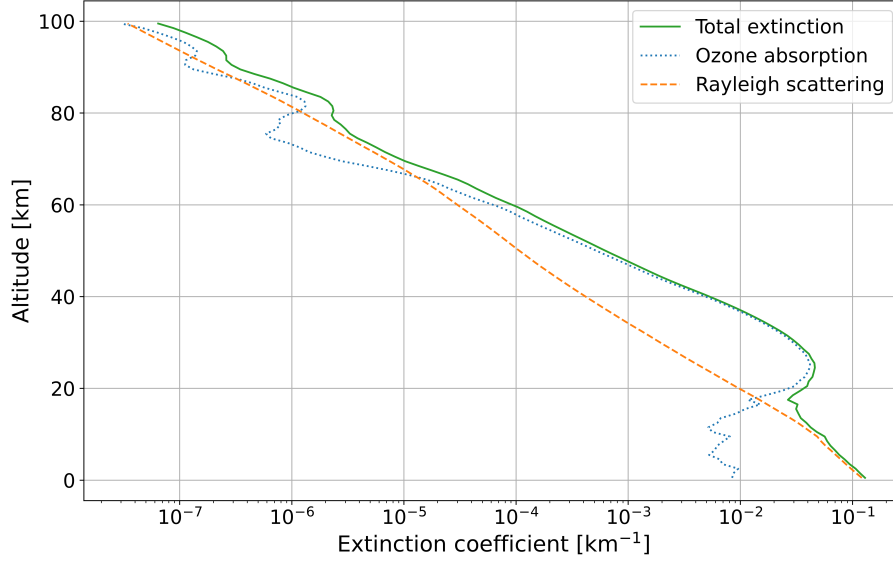


Figure 3.6: Profiles of the Rayleigh scattering coefficient (orange dashed line), ozone absorption coefficient (blue dotted line), and total extinction coefficient (green solid line) at $\lambda = 310$ nm.

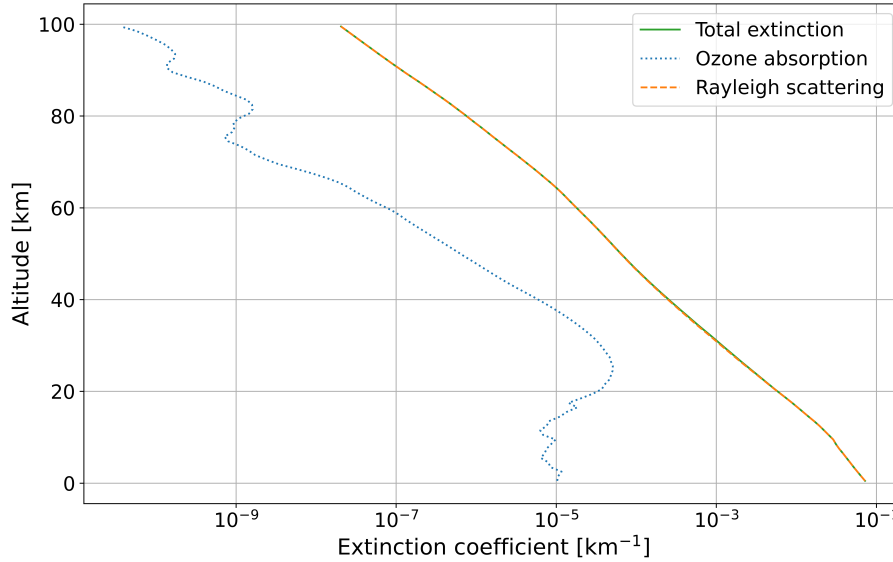


Figure 3.7: Profiles of the Rayleigh scattering coefficient (orange dashed line), ozone absorption coefficient (blue dotted line), and total extinction coefficient (green solid line) at $\lambda = 350$ nm.

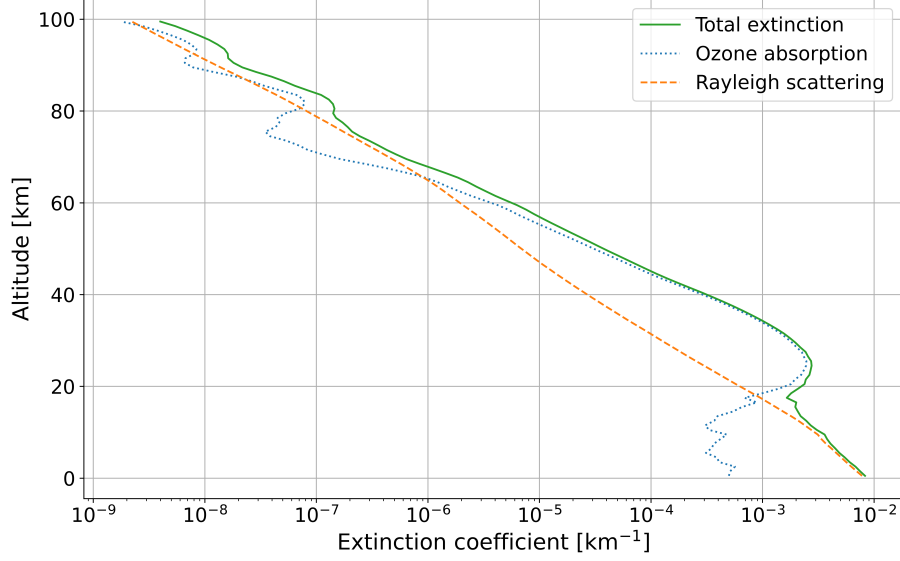


Figure 3.8: Profiles of the Rayleigh scattering coefficient (orange dashed line), ozone absorption coefficient (blue dotted line), and total extinction coefficient (green solid line) at $\lambda = 600$ nm.

3.4 Intersections

Once the osculating-sphere geometry and the atmospheric discretization have been constructed, the next step of the RTM consists in determining how propagation rays intersect the atmospheric layers. These intersections constitute a central geometric component of the radiative transfer calculation since they define the atmospheric segments over which extinction contributions must subsequently be evaluated.

In the present implementation, the atmospheric layers are represented by concentric spherical cells centered on the osculating-sphere center $\mathbf{C}_{\alpha_{\text{LOS}}^{\text{T}}}$. Consequently, determining the atmospheric path traversed by a ray reduces to computing the intersections between a straight propagation ray and a set of concentric spheres.

Consider a line originating from position $\vec{r}_0$ that may be parameterized as

$$\vec{r}(s) = \vec{r}_0 + \hat{u}s, \quad (3.24)$$

where $\hat{u}$ denotes the viewing direction and s is the path coordinate measured along the line. Of course, as shown in Figure 3.9, the instrument LOS constitutes one important example of such a propagation ray, which explains why the notation introduced previously has been retained here. However, the present formulation should be regarded as completely general and applies to any straight propagation path considered in the RTM.

For a spherical atmospheric shell of radius R_i , centered at $\mathbf{C}_{\alpha_{\text{LOS}}^{\text{T}}}$, the intersection condition is given by

$$\|\vec{r}_0' + \hat{u}s\|^2 = R_i^2, \quad (3.25)$$

where

$$\vec{r}_0' = \vec{r}_0 - \mathbf{C}_{\alpha_{\text{LOS}}^{\text{T}}}. \quad (3.26)$$

is the position vector shifted relative to the center of the osculating sphere.

Expanding the intersection condition leads to the quadratic equation

$$s^2 + 2(\vec{r}'_0 \cdot \hat{u})s + (\|\vec{r}'_0\|^2 - R_i^2) = 0. \quad (3.27)$$

The corresponding discriminant is therefore

$$\Delta_i = 4(\vec{r}'_0 \cdot \hat{u})^2 - 4(\|\vec{r}'_0\|^2 - R_i^2). \quad (3.28)$$

Whenever $\Delta_i < 0$, no intersection exists between the propagation ray and the considered atmospheric shell. Otherwise, the two intersection path coordinates are obtained analytically as

$$s_i^\pm = -(\vec{r}'_0 \cdot \hat{u}) \pm \frac{\sqrt{\Delta_i}}{2}. \quad (3.29)$$

This analytical formulation is applied to all atmospheric shell boundaries. The resulting intersection coordinates are subsequently sorted along the propagation direction, and only positive values are retained since negative path coordinates correspond to intersections located opposite to the viewing direction, as illustrated in Figure 3.9.

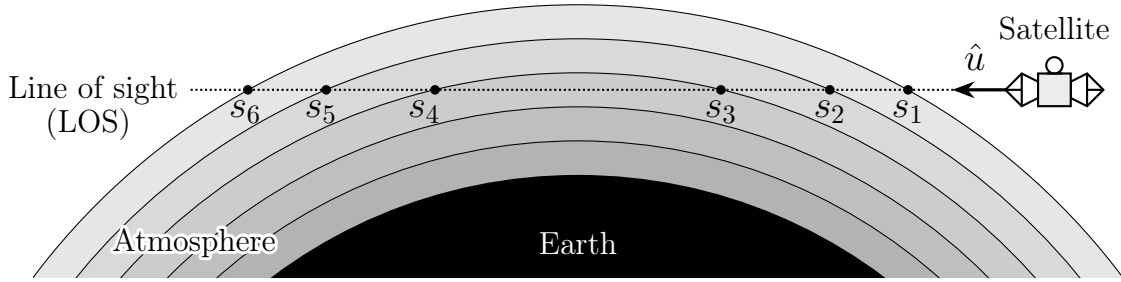


Figure 3.9: Illustration of the intersections between the instrument LOS and the concentric spherical shell boundaries defining the atmospheric discretization. The ordered intersection coordinates $\{s_i\}_{i=1}^6$ delimit atmospheric segments entirely contained within individual spherical cells.

3.5 Calculation of optical thickness

The attenuation of radiation along atmospheric propagation paths is governed by the optical thickness. In the present single-scattering RTM, optical thickness calculations are required for both the solar path between the top of the atmosphere and a scattering point, and for the observer path between the scattering point and the satellite.

As described previously, atmospheric quantities are assumed to vary linearly with altitude between adjacent layer midpoints. Consequently, before evaluating the optical thickness, each propagation ray is subdivided into atmospheric segments using the intersections with concentric spherical shells associated with the altitude grid of the layer midpoints (3.21). The lower and upper atmospheric boundaries at 0 km and 100 km are added explicitly.

Following the procedure described in the previous section, all positive intersection coordinates are first computed and sorted along the propagation direction. Consecutive intersections then define atmospheric segments bounded by the path coordinates (s_j, s_{j+1}) , as illustrated in Figure 3.10. Within each segment, the extinction coefficient is assumed to vary linearly with altitude, allowing the optical-thickness integral to be evaluated analytically using the formulation derived in [42].

The optical-thickness contribution associated with segment j is therefore written as

$$\tau_j \equiv \tau(s_j, s_{j+1}) = \int_{s_j}^{s_{j+1}} k(s) ds, \quad (3.30)$$

where $k(s)$ denotes the extinction coefficient along the propagation path.

Within the considered segment, the extinction coefficient is represented by a linear function of the altitude, or equivalently of the radial distance r ,

$$k(r) = A_j r + B_j, \quad (3.31)$$

with

$$A_j = \frac{k_{j+1} - k_j}{r_{j+1} - r_j}, \quad (3.32)$$

$$B_j = k_j - A_j r_j. \quad (3.33)$$

Here, $r_j \equiv r(s_j)$ and $r_{j+1} \equiv r(s_{j+1})$ denote the radial distances of the segment endpoints relative to the osculating-sphere center, while $k_j \equiv k(s_j)$ and $k_{j+1} \equiv k(s_{j+1})$ are the corresponding extinction coefficients from the atmospheric profile.

Using the analytical derivation presented in Appendix B of [42], the optical thickness of segment j becomes

$$\begin{aligned} \tau_j = B_j \Delta s_j + \frac{A_j}{2} \left[\Delta s_j r_{j+1} + r_j (r_{j+1} - r_j) \cos \theta_j \right. \\ \left. + r_j^2 \sin^2 \theta_j \ln \left(\frac{r_{j+1} + \Delta s_j + r_j \cos \theta_j}{r_j (1 + \cos \theta_j)} \right) \right], \end{aligned} \quad (3.34)$$

where

$$\Delta s_j = s_{j+1} - s_j. \quad (3.35)$$

Indicated in Figure 3.10, the angle θ_j denotes the angle between the LOS in the direction of propagation and the local zenith direction passing through the point located at radial distance r_j from the center of the Earth.

For nearly vertical inward propagation paths corresponding to $\cos \theta_j \rightarrow -1$, the logarithmic term becomes undetermined. In this limit, the implementation reverts to the trapezoidal approximation

$$\tau_j = \frac{(k_j + k_{j+1}) \Delta s_j}{2}. \quad (3.36)$$

The total optical thickness along the propagation ray is finally obtained by summing the contributions from all atmospheric segments,

$$\tau = \sum_j \tau_j. \quad (3.37)$$

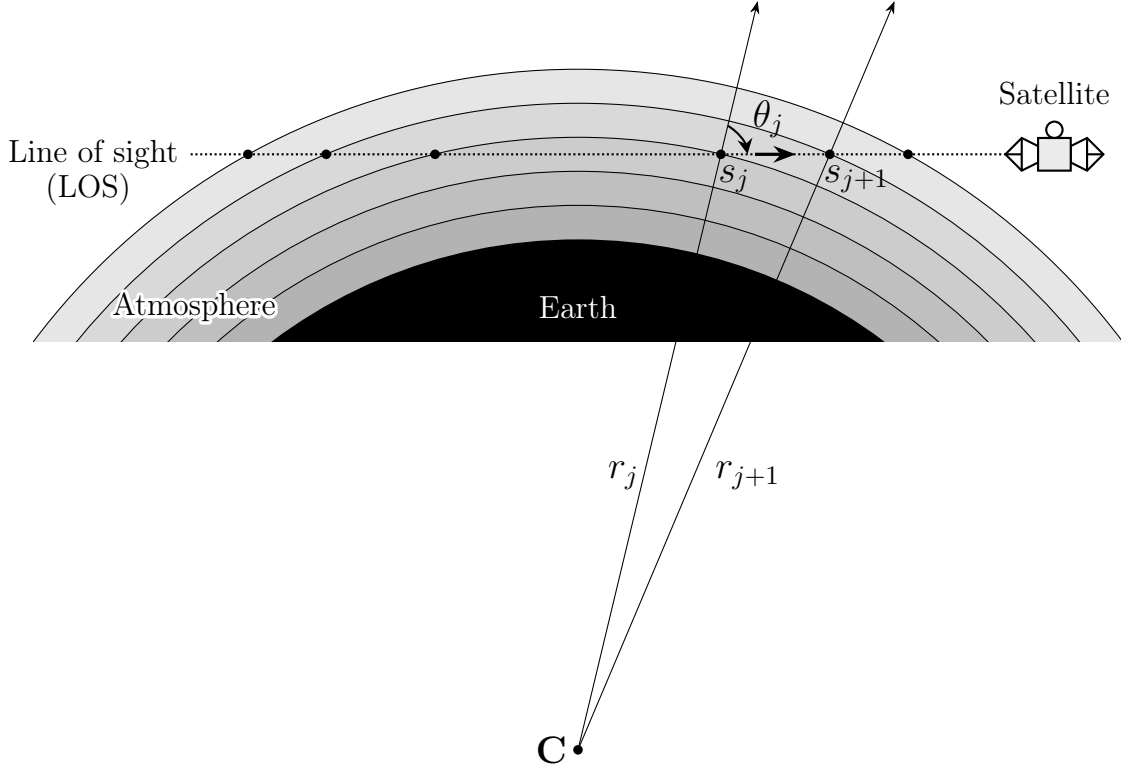


Figure 3.10: Illustration of the subdivision of a propagation ray into atmospheric segments using intersections with concentric spherical shell associated with the altitude grid of the layer midpoints. Consecutive intersection coordinates (s_j, s_{j+1}) define a segment over which the extinction coefficient is assumed to vary linearly with altitude and the optical-thickness integral is evaluated analytically.

3.6 Calculation of single-scattered radiance

3.6.1 Numerical evaluation

The single-scattered radiance is evaluated by integrating the scattering contributions along the instrument LOS via Equation (2.50). In principle, this requires considering an infinite number of scattering points along the propagation path. In practice, the LOS is discretized into a finite number of atmospheric segments obtained from the intersections between the LOS and the concentric spherical-shell boundaries defining the atmospheric grid. For most atmospheric segments, the single scatter source term is evaluated at the segment midpoint. However, the segment containing the tangent point generally corresponds to a much longer atmospheric path length. In this region, the tangent segment is therefore further subdivided using a fixed spatial sampling step $\Delta s = 10$ km, as shown in Figure 3.11.

The single-scattered radiance observed at position $\vec{r}_0$ in the direction $\hat{\Omega}$ is then approximated by the discrete path integral

$$I(\vec{r}_0, \hat{\Omega}) = F(\hat{\Omega}_\odot) \sum_{s \in \text{LOS}} e^{-\tau(\text{Sun}, s)} k_{\text{scatt}}(s) \bar{p}(s, \Theta) e^{-\tau(s, 0)} \Delta s. \quad (3.38)$$

For each discretization point along the LOS, a solar ray is traced from the top of the atmosphere to the scattering location in order to evaluate the attenuation $e^{-\tau(\text{Sun}, s)}$ of the incoming solar radiation before scattering into the observer direction. The locally scattered contribution is subsequently attenuated through $e^{-\tau(s, 0)}$ along the observer path before reaching the satellite. The optical thicknesses $\tau(\text{Sun}, s)$ and $\tau(s, 0)$ are evaluated using the analytical formulation described in the previous section.

In order to remove the direct dependence on the incident solar irradiance, the limb-scattered radiance is normalized by the solar flux at the top of the atmosphere. In the present work, the incident solar irradiance is set to unity, i.e. $F(\hat{\Omega}_{\odot}) = 1 \text{ W m}^{-2} \text{ nm}^{-1}$, such that the resulting Sun-normalized radiances are expressed in units of sr^{-1} .

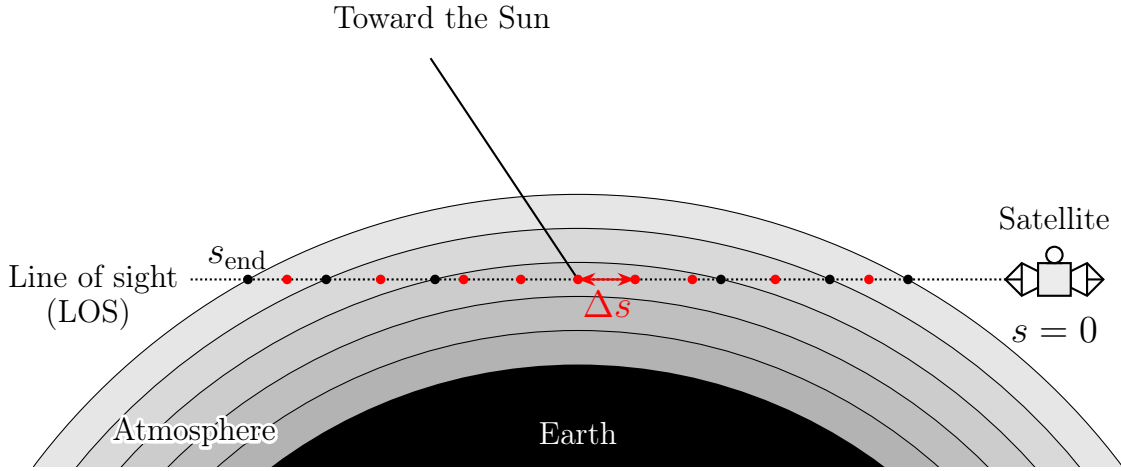


Figure 3.11: Illustration of the LOS discretization used for the single-scattering radiance calculation. The intersections between the LOS and the concentric spherical-shell boundaries define atmospheric segments within which the source term is evaluated. In the tangent region, where the optical path is longest, the LOS is further subdivided using a fixed spatial sampling step $\Delta s = 10 \text{ km}$.

3.6.2 Variations with wavelength

Using the implementation described in the previous sections, it is now possible to compute the single-scattered radiance associated with a given instrument LOS, or equivalently with a given tangent altitude. By tracing multiple LOS corresponding to different tangent altitudes, limb radiance profiles may therefore be obtained.

In all simulations presented hereafter, the satellite is positioned at

$$(\varphi_0, \lambda_0, h_0) = (20^\circ, 30^\circ, 840 \text{ km}). \quad (3.39)$$

The latitude and longitude were chosen arbitrarily, whereas the satellite altitude was selected close to that of the Suomi National Polar-orbiting Partnership (Suomi-NPP) satellite carrying the OMPS-LP instrument, whose observations will be used in the final part of this work to retrieve high-altitude temperatures.

The LOS azimuth angle at the satellite position is also chosen subjectively as

$$\alpha_{\text{LOS}}^0 = 0^\circ. \quad (3.40)$$

The atmosphere is then scanned using 100 LOS uniformly distributed between tangent altitudes of 1 km and 99 km.

Since the beginning of the radiative-transfer development, the wavelength dependence of the radiance expressions has remained implicit. However, the measured radiance strongly depends on wavelength because the atmospheric extinction coefficients associated with Rayleigh scattering k_{scatt} and ozone absorption k_{abs} vary significantly across the spectrum (see Figures 3.6, 3.7, and 3.8).

Figure 3.12 presents normalized limb radiance profiles at $\lambda = 310$ nm, 350 nm, and 600 nm. The solar zenith and azimuth angles at the satellite position were arbitrarily fixed to

$$(\theta_{\odot}^0, \phi_{\odot}^0) = (30^\circ, 45^\circ). \quad (3.41)$$

The dependence of the radiance profiles on the solar geometry will be discussed in the next subsection.

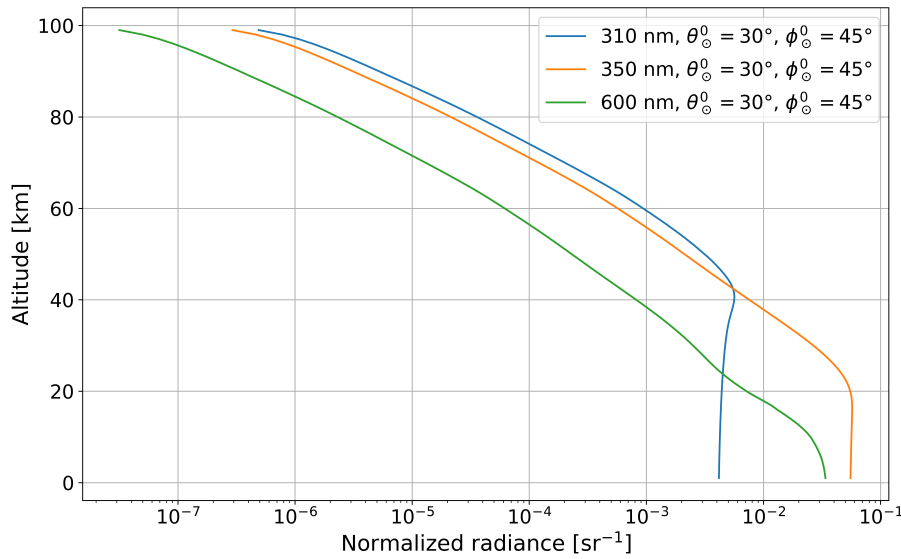


Figure 3.12: Logarithmic-scale normalized limb radiance profiles at $\lambda = 310$ nm (blue line), $\lambda = 350$ nm (orange line), and $\lambda = 600$ nm (green line), for $\theta_{\odot}^0 = 30^\circ$ and $\phi_{\odot}^0 = 45^\circ$.

Figure 3.12 highlights substantial differences between the radiance profiles at different wavelengths. In all cases, the radiance initially increases nearly exponentially as the tangent altitude decreases. In this optically thin regime, the measured radiance is essentially proportional to the number of scatterers along the LOS. Since the atmospheric number density increases nearly exponentially toward lower altitudes, the radiance follows a similar behavior. At sufficiently low tangent altitudes, however, the atmosphere progressively becomes optically thick along the LOS. The attenuation of both the incoming solar beam and the scattered radiation then compensates for the increase in air density, leading to a progressive saturation, or “knee”, in the limb radiance profile. The transition altitude between the exponential and saturated regimes strongly depends on wavelength.

At 310 nm, the transition occurs near 45 km. At this wavelength, both Rayleigh scattering and ozone absorption are strong. As a result, photons originating from deeper atmospheric layers are strongly attenuated before reaching the observer, producing an early saturation of the radiance profile.

At 350 nm, ozone absorption becomes much weaker, while the Rayleigh extinction is smaller by a factor of $(350/310)^4 \sim 1.6$. Consequently, the atmosphere remains optically thin down to lower altitudes, and the transition toward saturation occurs near 20–25 km. It is therefore possible to observe deeper into the atmosphere along the tangent path.

Finally, at 600 nm, the total optical thickness is considerably smaller than at shorter wavelengths. The radiance therefore continues to increase almost exponentially over most of the altitude range, with only limited saturation at low tangent altitudes.

3.6.3 Variations in solar angles

In addition to their wavelength dependence, limb radiance profiles also depend on the position of the Sun and therefore on the illumination geometry of the scattering points along the LOS. A modification of the solar geometry directly affects both the scattering angle Θ , and consequently the effective Rayleigh phase function $\bar{p}(\Theta)$, as well as the optical path traversed by incoming solar photons before reaching the scattering point. Since Rayleigh scattering preferentially occurs in the forward and backward directions, configurations associated with smaller or larger scattering angles generally produce larger radiances than configurations close to $\Theta \approx 90^\circ$, for which the phase function reaches a minimum. In addition, increasing the solar zenith angle enhances atmospheric attenuation along the solar path. In this work, solar zenith angles larger than 90° are not considered because, in this case, the direct solar beam would intersect atmospheric layers located below the tangent altitude, which is undesired.

Figures 3.13 and 3.14 present normalized limb radiance profiles obtained for four solar zenith and solar azimuth angles, respectively. In both cases, the wavelength was fixed to $\lambda = 600$ nm. Similar behaviors are obtained at other wavelengths.

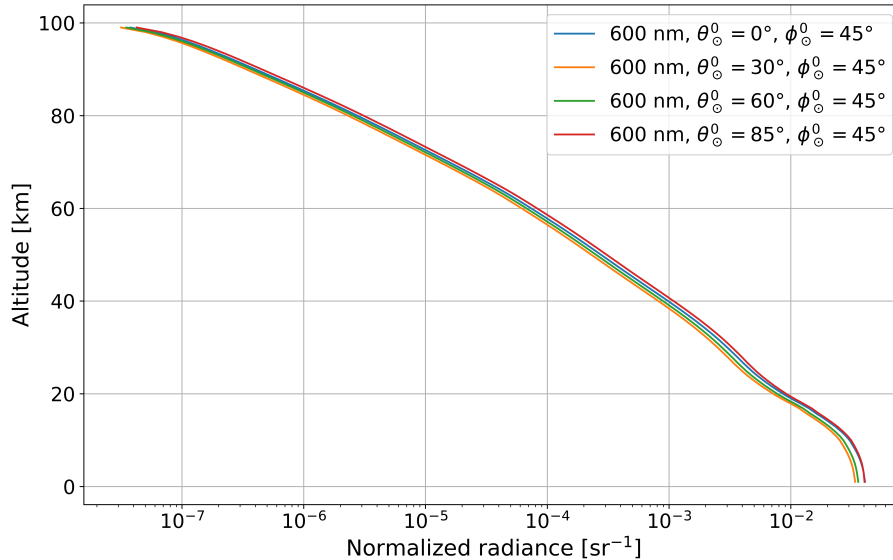


Figure 3.13: Logarithmic-scale normalized limb radiance profiles at $\lambda = 600$ nm for $\theta_{\odot}^0 = 0^\circ, 30^\circ, 60^\circ, 85^\circ$, with $\phi_{\odot}^0 = 45^\circ$.

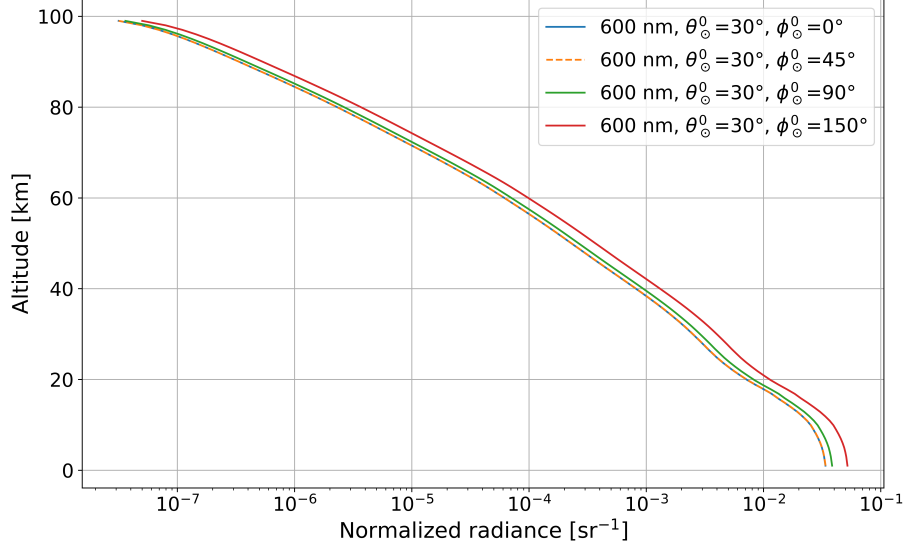


Figure 3.14: Logarithmic-scale normalized limb radiance profiles at $\lambda = 600$ nm for $\phi_{\odot}^0 = 0^\circ, 45^\circ, 90^\circ, 150^\circ$, with $\theta_{\odot}^0 = 30^\circ$.

3.6.4 Validation with SASKTRAN2

In order to validate the RTM developed in this work, the simulated limb-scattered radiance profiles are compared with those obtained using SASKTRAN2.

SASKTRAN is a radiative transfer framework originally developed at the University of Saskatchewan for the analysis of limb-scatter satellite measurements, notably from the OSIRIS instrument [29]. The model was specifically designed to provide accurate radiative transfer calculations in spherical geometry while remaining computationally efficient enough for limb-scatter retrievals. Comparisons in [29] have shown that SASKTRAN simulations agree well with both reference RTMs and satellite observations over a wide range of viewing geometries and atmospheric conditions. SASKTRAN2 is a complete rewrite of the original framework, providing better computational performance together with an improved Python interface [52].

The present model is therefore compared against SASKTRAN2 using the same atmospheric configuration, including only Rayleigh scattering and ozone absorption. The main difference between the two implementations lies in the definition of the inputs. In the present RTM, the viewing and solar geometries are specified at the satellite position, whereas SASKTRAN2 defines the geometry relative to the tangent point. Several transformations were therefore necessary to ensure consistency between the input parameters used by both models.

A comparison of the normalized limb radiance profiles is shown in Figure 3.15 for the same three wavelengths considered previously, namely $\lambda = 310$ nm, 350 nm, and 600 nm. The solar geometry was fixed to the default configuration defined by (3.41). Excellent agreement is observed between both models over the full tangent-altitude range and for all considered wavelengths. In order to quantify the differences more precisely, the *relative radiance difference* between the two models is computed as

$$\frac{I_{\text{RTM}} - I_{\text{SASKTRAN2}}}{I_{\text{SASKTRAN2}}}, \quad (3.42)$$

where I_{RTM} denotes the radiance obtained with the present model and $I_{\text{SASKTRAN2}}$ the radiance computed with SASKTRAN2.

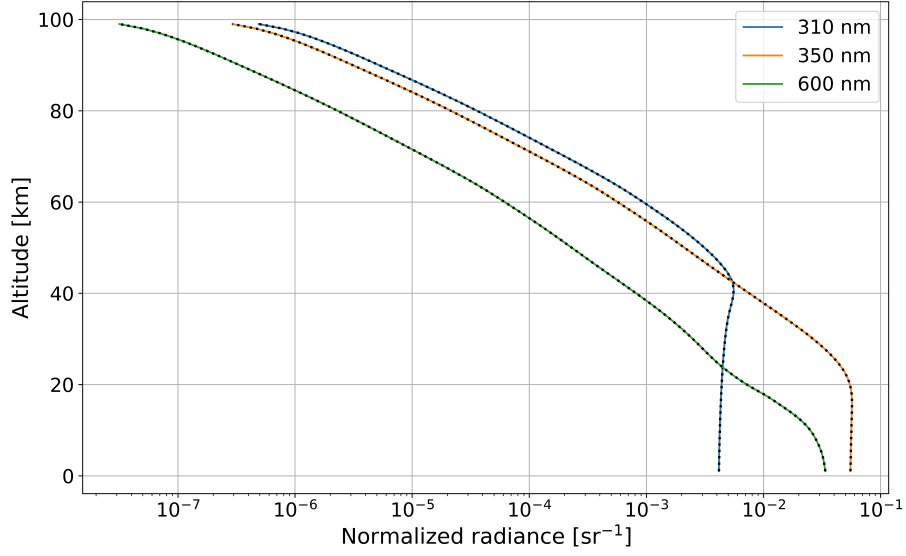


Figure 3.15: Comparison between normalized limb radiance profiles computed with the present model (solid lines) and with SASKTRAN2 (dotted lines) at $\lambda = 310$ nm (blue), $\lambda = 350$ nm (orange), and $\lambda = 600$ nm (green), for $\theta_{\odot}^0 = 30^\circ$ and $\phi_{\odot}^0 = 45^\circ$.

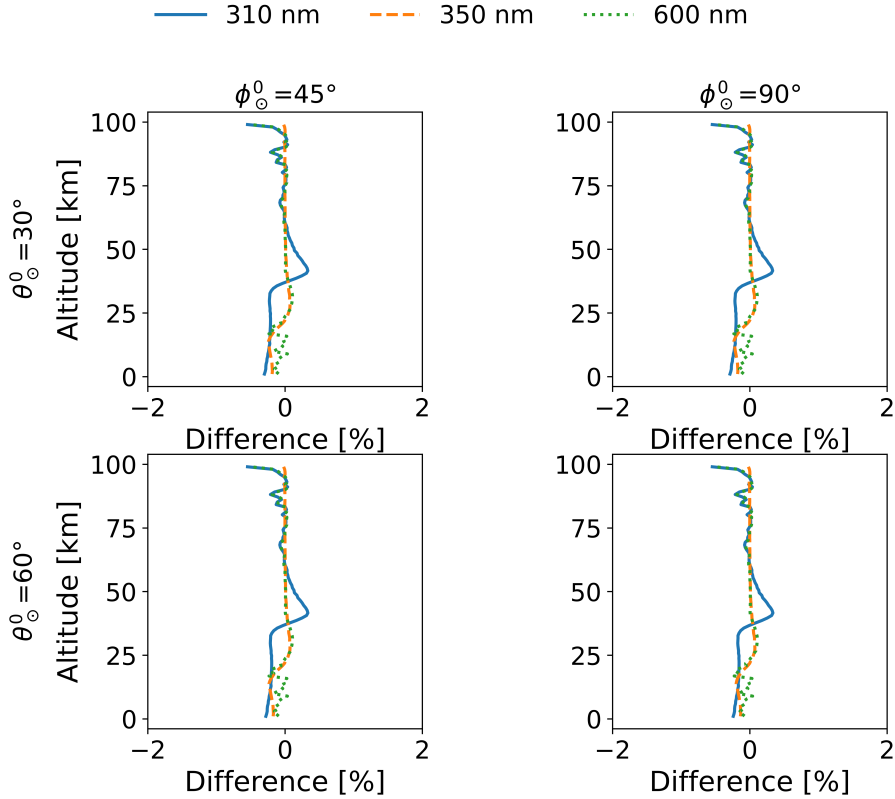


Figure 3.16: Relative differences between normalized limb radiance profiles computed with the present model and with SASKTRAN2 for four solar geometries, at $\lambda = 310$ nm (blue solid line), $\lambda = 350$ nm (orange dashed line), and $\lambda = 600$ nm (green dotted line).

As shown in Figure 3.16, the relative differences remain below approximately 1% for all tested solar geometries and wavelengths. Such agreement is expected since the present implementation was strongly inspired by the methodologies developed within the SASKTRAN framework. Nevertheless, the comparison confirms the correct implementation of the present single-scattering RTM. The validated model will therefore be used in the next chapter for the retrieval of middle atmospheric temperatures from limb-scatter measurements.

3.6.5 Impact of multiple scattering on radiance simulations

This final section presents a qualitative comparison between single-scattering simulations from the present model and multiple-scattering simulations from SASKTRAN2. The multiple-scattering calculations in SASKTRAN2 are performed using the *successive orders of scattering method* [29, 52]. This approach solves the radiative transfer equation iteratively by successively adding higher scattering orders to the source function. A key advantage is that the method fully accounts for the spherical geometry of the atmosphere, making it well suited for limb-viewing applications. However, it is computationally demanding, requiring significant memory and processing time.

Figure 3.17 shows normalized limb radiance profiles for the same wavelengths as before, namely $\lambda = 310$ nm, 350 nm, and 600 nm, comparing the single-scattering results from the present model with the multiple-scattering results from SASKTRAN2. As expected, multiple scattering leads to systematically higher radiances, since additional scattering events contribute to the observed signal beyond the first-order approximation. A notable result is that the overall shape of the limb radiance profiles remains very similar. This indicates that while multiple scattering increases the absolute magnitude of the signal, it does not modify its vertical structure. The multiple-scattering solution can thus be interpreted as a scaled version of the single-scattering solution, with a nearly uniform positive offset in radiance.

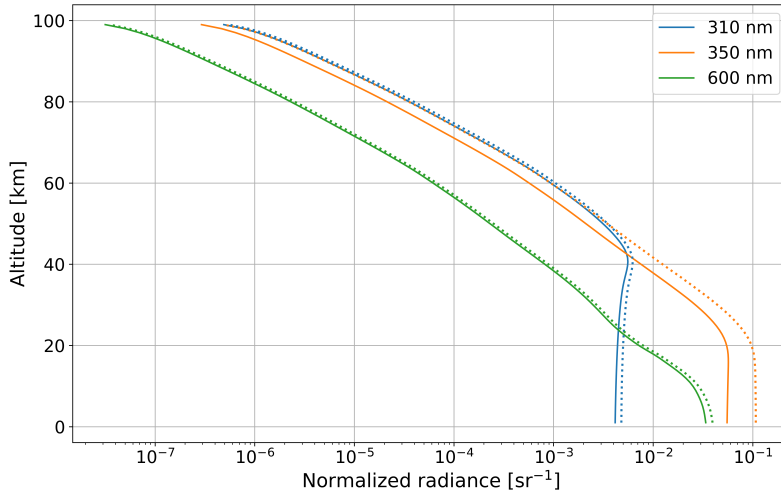


Figure 3.17: Comparison between normalized limb radiance profiles computed with the present single-scattering model (solid lines) and with SASKTRAN2 (dotted lines) using the successive orders of scattering method at $\lambda = 310$ nm (blue), $\lambda = 350$ nm (orange), and $\lambda = 600$ nm (green), for $\theta_{\odot}^0 = 30^\circ$ and $\phi_{\odot}^0 = 45^\circ$.

Chapter 4

Temperature retrieval

This chapter addresses the objective of retrieving the temperature in the middle atmosphere from limb-scattering satellite observations, such as those provided by the OMPS-LP instrument. The previous chapters focused on the theoretical development and numerical implementation of a RTM under the single-scattering approximation. The purpose of the present chapter is to show how this model can be combined with satellite observations in order to infer atmospheric temperature profiles.

4.1 The inverse problem

Physics aims at describing and understanding natural phenomena through mathematical models. In many applications, a theory is first established in order to predict observable quantities from a known physical state. This approach is referred to as the *forward problem*. In atmospheric remote sensing, the forward problem consists in computing the radiance measured by an instrument for a given atmospheric state. This is precisely the role of the RTM developed in the previous chapters. Under a set of simplifying assumptions, the model computes the radiance associated with prescribed atmospheric parameters such as temperature, pressure, and species number densities. In this context, the RTM acts as a *forward model*.

The objective of this chapter is fundamentally different. Instead of predicting the measurements from a known atmosphere, the goal is to infer the atmospheric state directly from the measurements themselves. This constitutes the *inverse problem*, commonly referred to as a *retrieval problem*.

If the atmospheric state were perfectly known, the forward model would be able to reproduce the signal measured by the instrument. The retrieval problem therefore consists in solving the opposite question: determining which atmospheric state most likely produced the observed radiances. In practice, however, this inversion is not straightforward. The relationship between the atmospheric state and the measured signal is generally nonlinear, while the observations themselves are affected by measurement uncertainties. As a consequence, the inverse problem cannot usually be solved analytically and requires inversion techniques. This forward-inverse relationship is illustrated schematically in Figure 4.1, where the main quantities involved and the retrieval algorithm will be formally defined in the Section 4.3.

Up to this point, the discussion has remained deliberately general by referring to atmospheric state. In the present work, however, the quantity of interest is specifi-

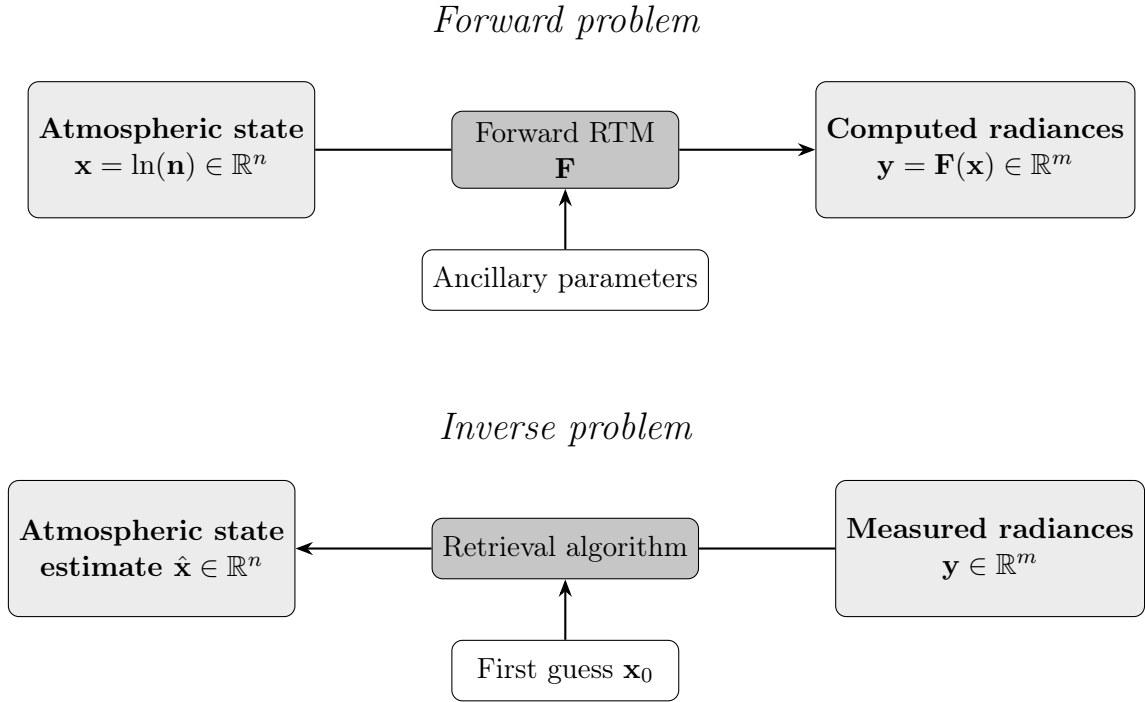


Figure 4.1: Schematic representation of the forward and inverse modeling framework. The forward RTM $\mathbf{F}$ maps the atmospheric state vector $\mathbf{x}$ to the radiances $\mathbf{y}$ given other parameters. The inverse problem seeks to estimate the atmospheric state from measurements using a retrieval algorithm initialized with a first-guess state $\mathbf{x}_0$.

cally the atmospheric temperature. The difficulty arises from the fact that the RTM does not depend explicitly on temperature. Instead, the temperature dependence is implicitly contained in the air number density, which governs the Rayleigh scattering contribution to the measured radiance. Consequently, the temperature retrieval is performed in two successive steps. First, the air number density profile is retrieved from the measured radiances using inversion methods that will be introduced later in this chapter. Second, the temperature profile is derived from the retrieved air number density by combining the ideal gas law with the hydrostatic equilibrium equation relating pressure, density, and temperature.

For clarity, the temperature retrieval methodology will first be presented by describing how temperature can be derived from the retrieved air number density before introducing the inversion procedure itself.

4.2 Temperature retrieval from air number density

Assuming the air number density profile $n(h)$ is known¹, the atmospheric temperature profile can be derived by combining the ideal gas law with the hydrostatic equilibrium equation. The procedure followed here is closely related to the approach originally developed by Hauchecorne and Chanin [53] for Rayleigh lidar temperature retrievals.

¹A notation change is introduced in this chapter for clarity. In the previous chapters, the air number density was denoted n_{air} . From now on, the simpler notation n is used, such that $n \equiv n_{\text{air}}$.

4.2.1 Physical framework

The ideal gas law, established by Émile Clapeyron in 1834, relates pressure, number density, and temperature for a gas assumed to behave ideally. An ideal gas is a theoretical gas composed of non-interacting particles undergoing perfectly elastic collisions. Although real atmospheric gases do not strictly satisfy these assumptions, the ideal gas approximation remains remarkably accurate throughout most of the atmosphere.

Assuming that air behaves as an ideal gas mixture, the equation of state can be written as

$$P(h) = n(h)k_B T(h), \quad (4.1)$$

where P is the atmospheric pressure, n the air number density, k_B the Boltzmann constant, and T the absolute atmospheric temperature. All these atmospheric quantities depend on altitude h .

The second fundamental relation is the hydrostatic equilibrium equation,

$$dP(h) = -g(h)n(h)m(h)dh, \quad (4.2)$$

where g is the local gravitational acceleration and m the mean molecular mass of air. This equation expresses the fact that the pressure at a given altitude is caused by the weight of the atmospheric column above.

The molecular mass can itself be expressed as

$$m(h) = \frac{M_{\text{air}}(h)}{N_A}, \quad (4.3)$$

where M_{air} is the molar mass of air and $N_A = 6.022\,140\,76 \times 10^{23} \text{ mol}^{-1}$ is Avogadro number.

Combining the ideal gas law with the hydrostatic equilibrium equation yields

$$T(h) = \frac{1}{n(h)} \left(n_0 T_0 - \frac{1}{k_B} \int_{h_0}^h g(h')n(h')m(h')dh' \right), \quad (4.4)$$

where n_0 and T_0 denote the air number density and temperature at a reference altitude h_0 .

Equation (4.4) shows that the atmospheric temperature profile can be reconstructed from the air number density profile provided that a reference temperature is known. In the present work, the reference altitude is chosen near the top of the atmosphere, currently fixed at 100 km. The temperature retrieval is therefore performed from the top to the bottom of the atmosphere.

Two important properties emerge from Equation (4.4). Multiplying the number density profile by a constant scaling factor does not significantly modify the retrieved temperature profile. Consequently, the latter only depends on the shape of the air number density profile, and not on its magnitude. This scaling invariance provides robustness against systematic errors [15].

Second, errors associated with the reference temperature decrease rapidly with decreasing altitude. Since atmospheric density increases exponentially toward lower altitudes, the influence of the upper boundary condition progressively vanishes during the downward integration, as will be illustrated in the following subsection. Conversely, performing the retrieval upward from the surface would amplify uncertainties with altitude. For this reason, temperature retrievals based on hydrostatic integration are naturally performed downward through the atmosphere.

4.2.2 Numerical conversion from air number density to temperature

In practice, Equation (4.4) must be discretized in order to be applied to atmospheric layers sampled on a finite altitude grid. The formulation adopted here follows Appendix A of Zawada et al. [15].

Integrating the hydrostatic equilibrium equation between two altitudes gives

$$P(h) = P_0 - \int_{h_0}^h g(h')n(h')m(h')dh', \quad (4.5)$$

or equivalently, between two consecutive grid points altitudes,

$$P_{j+1} - P_j \equiv \Delta P_j = - \int_{h_j}^{h_{j+1}} g(h')n(h')m(h')dh', \quad (4.6)$$

where the index $j = 0$ corresponds to the uppermost altitude. The atmospheric pressure can therefore be recursively computed downward from the reference altitude.

To evaluate the integral analytically, the number density is assumed to vary linearly between grid points, consistent with what was used by the RTM:

$$n(h) = n_j + \frac{n_{j+1} - n_j}{h_{j+1} - h_j}(h - h_j), \quad h \in [h_j, h_{j+1}]. \quad (4.7)$$

The molar mass of air is assumed constant with altitude and fixed to

$$M_{\text{air}} = 28.97 \text{ g mol}^{-1}, \quad (4.8)$$

while the gravitational acceleration is assumed to decrease quadratically with height according to

$$g(h) = g_0 \frac{R_E^2}{(R_E + h)^2}, \quad (4.9)$$

where $g_0 = 9.80665 \text{ m s}^{-2}$ is the gravitational acceleration at the Earth's surface and $R_E = 6371 \text{ km}$ is the mean Earth radius.

Substituting these expressions into Equation (4.6) yields

$$\Delta P_j = -R_E^2 m g_0 \int_{h_j}^{h_{j+1}} \frac{1}{(R_E + h')^2} \left[n_j + \frac{n_{j+1} - n_j}{h_{j+1} - h_j}(h' - h_j) \right] dh'. \quad (4.10)$$

Performing the integration analytically leads to

$$\Delta P_j = -R_E^2 m g_0 \left[\frac{n_j}{R_E + h_j} - \frac{n_{j+1}}{R_E + h_{j+1}} + \frac{n_{j+1} - n_j}{h_{j+1} - h_j} \ln \left(\frac{R_E + h_{j+1}}{R_E + h_j} \right) \right]. \quad (4.11)$$

The retrieval algorithm can therefore be summarized as follows. Starting from a reference temperature T_0 , the corresponding pressure at the upper boundary is first evaluated using the ideal gas law,

$$P_0 = n_0 k_B T_0. \quad (4.12)$$

The pressure profile is then recursively propagated downward using Equation (4.11). Finally, the temperature at each grid point can be evaluated with the ideal gas law:

$$T_j = \frac{P_j}{n_j k_B}. \quad (4.13)$$

4.2.3 Assessment of the temperature retrieval algorithm

The performance of the temperature retrieval algorithm is first evaluated under idealized conditions. To do so, the same air number density profile previously used in the forward RTM simulations of Section 3.6 is employed as input to the retrieval algorithm. In this test case, the density profile is assumed to be perfectly known, meaning that no inversion error is introduced.

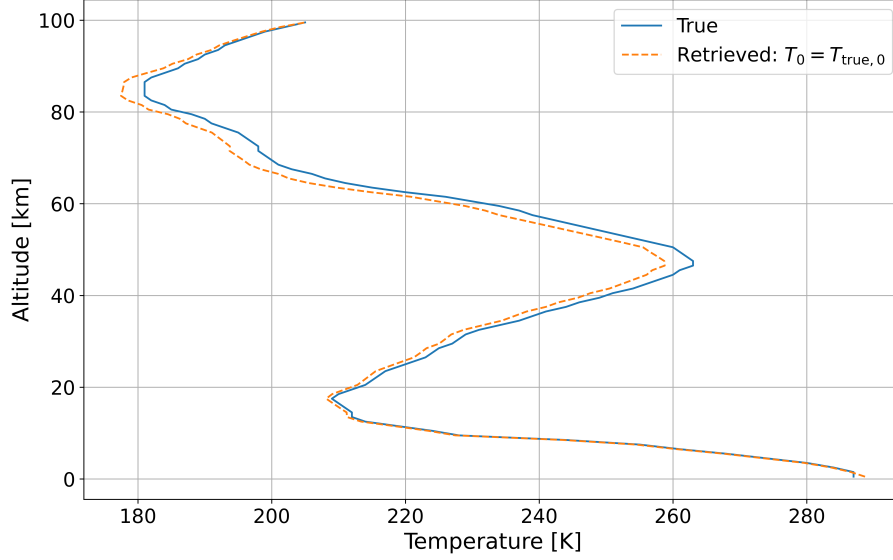


Figure 4.2: Comparison between the original atmospheric temperature profile (blue solid line) and the temperature profile retrieved from the corresponding air number density profile (orange dashed line).

Figure 4.2 compares the *retrieved* temperature profile with the *true* temperature profile used to generate the air number density profile. The same upper boundary temperature T_0 is imposed in both cases, such that the two profiles coincide at the top of the atmosphere. Small discrepancies remain throughout the profile. At first sight, these differences may appear surprising since the air number density was itself originally derived from the same temperature and pressure profiles through the ideal gas law. However, although these atmospheric fields satisfy the ideal gas law by construction, they are not necessarily fully consistent with hydrostatic equilibrium simultaneously. Indeed, the atmospheric profiles used here originate from atmospheric datasets and retrieval products rather than from an atmosphere analytically constrained to satisfy both relations exactly. The differences observed in Figure 4.2 therefore most likely reflect small deviations from perfect hydrostatic equilibrium.

To verify this interpretation, the same retrieval algorithm is applied using pressure, temperature, and density profiles from the International Civil Aviation Organization (ICAO) Standard Atmosphere 1993 [54], which extends up to 80 km and is analytically constructed to satisfy both hydrostatic equilibrium and the ideal gas law.

As shown in Figure 4.3, the *retrieved* and reference (*true*) temperature profiles become indistinguishable when using the ICAO atmosphere. The discrepancies previously observed therefore disappear entirely, confirming the internal consistency and validity of the retrieval algorithm.

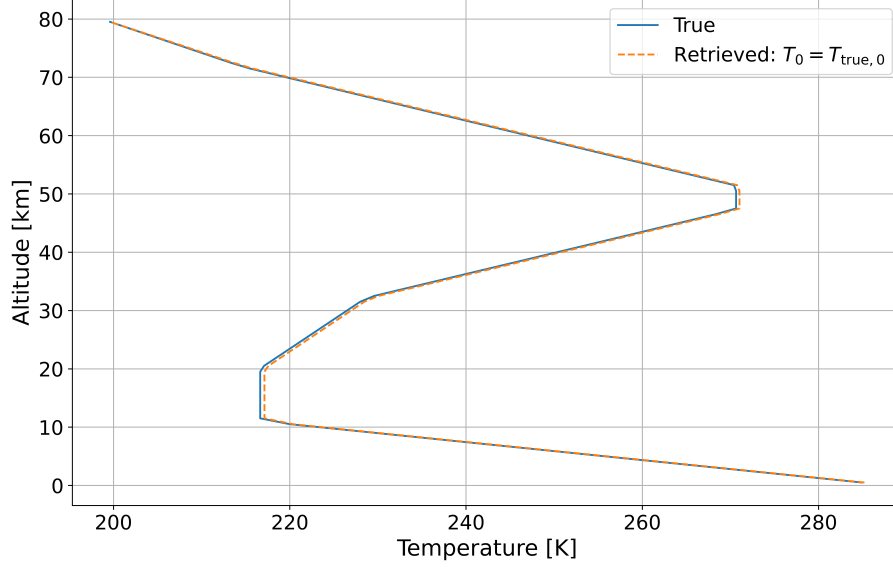


Figure 4.3: Comparison between the ICAO 1993 temperature profile (blue solid line) and the temperature profile retrieved from the corresponding ICAO air number density profile (orange dashed line).

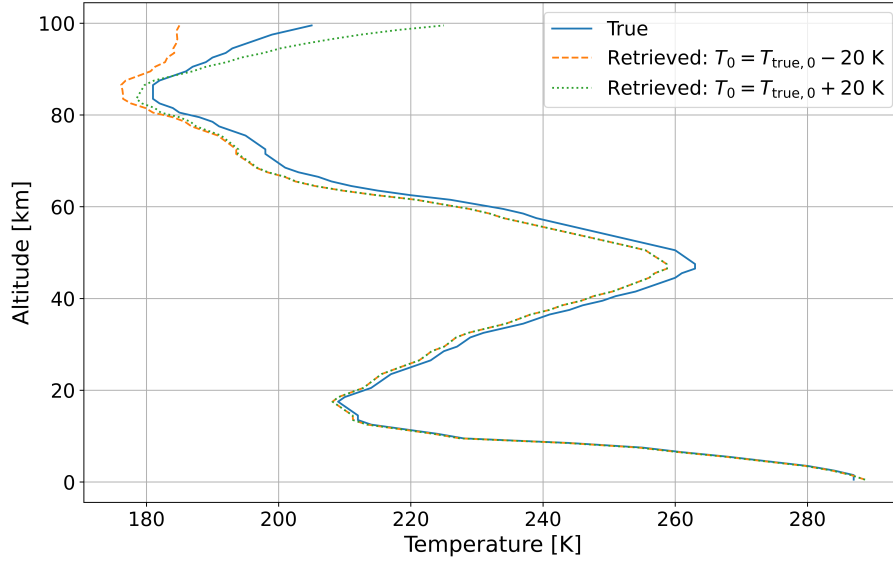


Figure 4.4: Retrieved temperature profiles obtained using upper boundary temperatures differing by 20 K (orange dashed line and green dotted line) from the true atmospheric temperature (blue solid line).

Finally, the sensitivity of the retrieval to the reference temperature is investigated. To this end, the upper boundary temperature T_0 is artificially perturbed by 20 K relative to the true atmospheric temperature. Figure 4.4 shows that the effect of the boundary condition rapidly vanishes with decreasing altitude. The retrieval progressively converges back toward the *true* temperature profile despite the initial temperature offset. This behavior directly results from the downward integration scheme and the exponential increase of atmospheric density toward lower altitudes.

This property is particularly advantageous in practice. Although the temperature near the top of the atmosphere is generally more uncertain, the associated

errors naturally decay during the downward integration. By contrast, an upward integration initiated from the surface would progressively amplify boundary-condition uncertainties with altitude.

4.3 Air number density retrieval

The previous section demonstrated that atmospheric temperature can be derived from the air number density profile through hydrostatic equilibrium and the ideal gas law. The next step therefore consists in retrieving the air number density itself from the measured limb-scattered radiances. This constitutes the core inverse problem of the present work. The notation used in this section follows the standard formalism introduced by Rodgers [55]. Further details on retrieval theory are given in [56].

4.3.1 Formulation of the inverse problem

In atmospheric remote sensing, the atmospheric state is intrinsically continuous with altitude. In practice, however, both the measurements and the retrieved quantities must be discretized onto a finite vertical grid. The atmospheric state is therefore represented by a finite-dimensional vector called the *state vector*,

$$\mathbf{x} = \{x_1, x_2, \dots, x_n\} \in \mathbb{R}^n, \quad (4.14)$$

where each element corresponds to a specific grid point altitude.

Similarly, the observations acquired by the instrument form the *measurement vector*,

$$\mathbf{y} = \{y_1, y_2, \dots, y_m\} \in \mathbb{R}^m, \quad (4.15)$$

where each component corresponds to a measurement associated with a given altitude. The dimensions m and n are not necessarily equal.

In the present work, the measurement vector consists of the measured limb-scattering radiance profile, while the state vector is chosen as the natural logarithm of the air number density profile,

$$\mathbf{x} = \ln(\mathbf{n}). \quad (4.16)$$

Using the logarithm rather than the number density itself is motivated by numerical stability. Since atmospheric density varies over several orders of magnitude throughout the atmosphere, working with logarithms prevents the largest values from dominating the inversion and improves the numerical conditioning of the problem.

The forward model establishes the relationship between the atmospheric state and the measured radiances. In compact form, this relationship can be written as

$$\mathbf{y} = \mathbf{F}(\mathbf{x}) + \boldsymbol{\varepsilon}, \quad (4.17)$$

where $\mathbf{F}$ denotes the forward RTM and $\boldsymbol{\varepsilon}$ represents the combined effect of measurement noise and modeling errors.

In practice, the forward model also depends on additional atmospheric and instrumental parameters that are assumed to be known and are therefore not retrieved. These ancillary parameters are omitted from the notation for simplicity.

4.3.2 Gauss–Newton algorithm

The objective of the retrieval is to determine the atmospheric state vector that best reproduces the measured radiances. In other words, the inverse problem consists in finding the state vector $\mathbf{x}$ such that the forward-modeled radiances $\mathbf{F}(\mathbf{x})$ match the observations $\mathbf{y}$ as closely as possible.

A standard approach for solving inverse problems consists in minimizing the difference between the observations and the radiances simulated by the forward model. This is commonly formulated as a least-squares minimization problem through the cost function

$$\mathcal{J}(\mathbf{x}) = \|\mathbf{y} - \mathbf{F}(\mathbf{x})\|^2 = (\mathbf{y} - \mathbf{F}(\mathbf{x}))^T (\mathbf{y} - \mathbf{F}(\mathbf{x})). \quad (4.18)$$

In principle, the solution could be obtained by evaluating the forward model for a very large number of possible atmospheric states and selecting the one producing the smallest residual. However, this approach involves a large number of evaluations of the forward model and rapidly becomes computationally prohibitive. Fortunately, the retrieval problem can be solved more efficiently using iterative optimization techniques.

The forward RTM is generally nonlinear with respect to the atmospheric state vector. To simplify the problem, the forward model can be linearized locally about a reference state $\mathbf{x}_0$ using a first-order Taylor expansion,

$$\mathbf{F}(\mathbf{x}) \approx \mathbf{F}(\mathbf{x}_0) + \mathbf{K}(\mathbf{x} - \mathbf{x}_0), \quad (4.19)$$

where $\mathbf{K}$ is the $m \times n$ *Jacobian matrix*, also called the *weighting function matrix*,

$$\mathbf{K} = \left. \frac{\partial \mathbf{F}(\mathbf{x})}{\partial \mathbf{x}} \right|_{\mathbf{x}_0}. \quad (4.20)$$

Once the forward model has been linearized, the inverse problem reduces locally to a linear least-squares problem. Starting from an initial estimate, or *first guess* $\mathbf{x}_0$, the atmospheric state can be iteratively improved using the Gauss–Newton algorithm.

The first estimate of the retrieved state is given by²

$$\hat{\mathbf{x}}^{(1)} = \mathbf{x}_0 + (\mathbf{K}^T \mathbf{K})^{-1} \mathbf{K}^T (\mathbf{y} - \mathbf{F}(\mathbf{x}_0)). \quad (4.21)$$

The Jacobian matrix is then recalculated around the updated state, and the procedure is repeated iteratively. The $(i + 1)$ -th iteration is therefore given by

$$\hat{\mathbf{x}}^{(i+1)} = \hat{\mathbf{x}}^{(i)} + \left(\mathbf{K}^{(i)T} \mathbf{K}^{(i)} \right)^{-1} \mathbf{K}^{(i)T} (\mathbf{y} - \mathbf{F}(\hat{\mathbf{x}}^{(i)})). \quad (4.22)$$

In this formulation, the a first guess $\mathbf{x}_0$ is identical to $\hat{\mathbf{x}}^{(0)}$. The iterations continue until some convergence criterion is satisfied.

²If the number of measurements equals the number of unknowns ($m = n$), then $\mathbf{K}$ is a square matrix and the problem could in principle be solved directly. In practice, however, inverse problems in atmospheric remote sensing are generally overdetermined ($m > n$). The retrieval therefore relies on the Moore–Penrose pseudo-inverse $(\mathbf{K}^T \mathbf{K})^{-1} \mathbf{K}^T$ rather than on the ordinary matrix inverse $\mathbf{K}^{-1}$.

4.3.3 Levenberg–Marquardt algorithm

Although the Gauss–Newton method converges rapidly when the current estimate is already close to the solution, it may become unstable when the problem is strongly nonlinear or when the first guess is too far from the optimum. To improve the robustness of the retrieval, the Gauss–Newton iteration is therefore modified using the Levenberg–Marquardt algorithm, introducing a damping term in Equation (4.22).

The iterative update then becomes

$$\hat{\mathbf{x}}^{(i+1)} = \hat{\mathbf{x}}^{(i)} + \left(\mathbf{K}^{(i)\text{T}} \mathbf{K}^{(i)} + \gamma^{(i)} \mathbf{D}^{(i)} \right)^{-1} \mathbf{K}^{(i)\text{T}} (\mathbf{y} - \mathbf{F}(\hat{\mathbf{x}}^{(i)})), \quad (4.23)$$

where $\gamma^{(i)}$ is the *damping parameter* and $\mathbf{D}^{(i)}$ is a diagonal matrix.

In the original formulation proposed by Levenberg, the damping matrix is chosen as the identity matrix,

$$\mathbf{D}^{(i)} = \mathbf{I}_n. \quad (4.24)$$

Marquardt [57] later introduced a scaled version in which the damping term is weighted by the diagonal of $\mathbf{K}^{\text{T}}\mathbf{K}$,

$$\mathbf{D}^{(i)} = \text{diag} \left(\mathbf{K}^{(i)\text{T}} \mathbf{K}^{(i)} \right). \quad (4.25)$$

The parameter $\gamma^{(i)}$ controls the behavior of the algorithm. For small values of $\gamma^{(i)}$, the damping term becomes negligible and the Levenberg–Marquardt iteration reduces to the standard Gauss–Newton method. Conversely, for large values of $\gamma^{(i)}$, the update approaches a steepest-descent step, producing smaller but more stable corrections.

In practice, the damping parameter is initially set to $\gamma^{(0)} = 1$ and adjusted dynamically during the iterations. After each update, the forward model is reevaluated and the cost function is recomputed. If the residual decreases, the iteration is accepted and the damping parameter is reduced by a factor of 3, allowing the algorithm to move closer to the Gauss–Newton regime and accelerate convergence. Otherwise, the iteration is rejected and the damping parameter is increased by a factor of 2 in order to enforce a more conservative step. This adaptive strategy considerably improves the stability of the retrieval, particularly during the first iterations when the solution may still be far from the minimum.

The iterations are terminated once the norm of the state update becomes sufficiently small,

$$\|\hat{\mathbf{x}}^{(i+1)} - \hat{\mathbf{x}}^{(i)}\| < \xi, \quad (4.26)$$

where ξ is a prescribed convergence threshold. In the present retrieval, a value of $\xi = 10^{-4}$ is used. A maximum of 10 iterations is imposed otherwise.

4.3.4 Jacobian matrix computation

Since the Levenberg–Marquardt algorithm requires repeated evaluations of the Jacobian matrix, its efficient computation is essential for the practical implementation of the retrieval.

The Jacobian matrix describes the sensitivity of the measured radiances to perturbations of the atmospheric state vector. More precisely, each element of the

Jacobian matrix represents the variation of a given radiance measurement induced by a perturbation of the atmospheric state at a specific grid point altitude,

$$K_{ij} = \frac{\partial I_i}{\partial x_j}, \quad (4.27)$$

where I_i denotes the radiance associated with the i -th LOS and x_j the j -th component of the state vector.

Since the retrieval is performed in logarithmic space, the weighting functions become

$$K_{ij} = \frac{\partial I_i}{\partial \ln(n_j)} = n_j \frac{\partial I_i}{\partial n_j}, \quad (4.28)$$

where n_j is the air number density at altitude level j .

A direct way to compute the Jacobian matrix consists in perturbing individually each atmospheric layer and evaluating the corresponding radiance variation using a finite difference technique:

$$K_{ij} \approx \frac{I_i(n_j + \delta n_j) - I_i(n_j)}{\delta}. \quad (4.29)$$

The perturbation δn_j is chosen as a small fraction of the local number density, that is $\delta n_j = 10^{-3} n_j$. Although conceptually simple, this approach requires one additional run of the forward RTM for every atmospheric grid cell. The computational cost therefore scales linearly with the number of retrieved parameters and rapidly becomes prohibitive.

To overcome this limitation, an analytic formulation of the Jacobian matrix can instead be derived. The derivation presented here closely follows the work of Zawada et al. [47].

Recall that the single-scattered radiance along the i -th LOS was approximated by the discrete path integral

$$I_i(\vec{r}_0, \hat{\Omega}) = \sum_{s \in \text{LOS}_i} e^{-\tau(\text{Sun}, s)} k_{\text{scatt}}(s) \bar{p}(s, \Theta) e^{-\tau(s, 0)} \Delta s. \quad (4.30)$$

The dependence of the radiance on the air number density appears through three distinct terms:

- the optical depth between the Sun and the scattering point $\tau(\text{Sun}, s)$,
- the local scattering extinction coefficient $k_{\text{scatt}}(s)$,
- the optical depth between the scattering point and the observer $\tau(s, 0)$.

Differentiating the radiance with respect to the number density therefore produces three separate contributions,

$$\begin{aligned} \frac{\partial I_i}{\partial n_j} = \sum_{s \in \text{LOS}_i} & \left[\frac{\partial e^{-\tau(\text{Sun}, s)}}{\partial n_j} k_{\text{scatt}}(s) e^{-\tau(s, 0)} \right. \\ & + e^{-\tau(\text{Sun}, s)} \frac{\partial k_{\text{scatt}}(s)}{\partial n_j} e^{-\tau(s, 0)} \\ & \left. + e^{-\tau(\text{Sun}, s)} k_{\text{scatt}}(s) \frac{\partial e^{-\tau(s, 0)}}{\partial n_j} \right] \bar{p}(s, \Theta) \Delta s. \end{aligned} \quad (4.31)$$

To proceed further, the discrete representation of the atmosphere used by the RTM must be specified. In the present model, the atmosphere is represented using linear interpolation between grid cells. The atmospheric number density profile can therefore be expressed as

$$n(h) = \sum_j n_j \mathcal{R}_j(h), \quad (4.32)$$

where $\mathcal{R}_j$ denotes the *basis function* associated with atmospheric layer j .

Since the RTM represents the atmosphere as a piecewise-linear function, the basis functions correspond to *triangular functions*, also known as *linear B-splines*,

$$\mathcal{R}_j(h) = \begin{cases} \frac{h - h_{j-1}}{h_j - h_{j-1}} & \text{if } h_{j-1} \leq h \leq h_j, \\ \frac{h_{j+1} - h}{h_{j+1} - h_j} & \text{if } h_j < h \leq h_{j+1}, \\ 0 & \text{otherwise.} \end{cases} \quad (4.33)$$

With this representation, perturbing the density at altitude level j only affects the atmosphere locally over the interval $[h_{j-1}, h_{j+1}]$.

The scattering extinction coefficient can then be written as

$$k_{\text{scatt}}(s) = \sigma_r n(s), \quad (4.34)$$

where σ_r is the Rayleigh scattering cross section. Its derivative with respect to n_j becomes

$$\frac{\partial k_{\text{scatt}}(s)}{\partial n_j} = \sigma_r \mathcal{R}_j(s). \quad (4.35)$$

Similarly, for the optical thickness between s_1 and s_2 ,

$$\frac{\partial (e^{-\tau(s_1, s_2)})}{\partial n_j} = -e^{-\tau(s_1, s_2)} \frac{\partial \tau(s_1, s_2)}{\partial n_j}, \quad (4.36)$$

with

$$\frac{\partial \tau(s_1, s_2)}{\partial n_j} = \int_{s_1}^{s_2} \mathcal{R}_j(s) ds. \quad (4.37)$$

Combining all contributions finally yields the analytic expression of the single scatter weighting function,

$$K_{ij} = n_j \sum_{s \in \text{LOS}_i} \left[\begin{array}{l} + \mathcal{R}_j(s) \\ - k_{\text{scatt}}(s) \int_{\text{Sun}}^s \mathcal{R}_j(s') ds' \\ - k_{\text{scatt}}(s) \int_s^0 \mathcal{R}_j(s') ds' \end{array} \right] \sigma_r e^{-\tau(\text{Sun}, s)} e^{-\tau(s, 0)} \bar{p}(s, \Theta) \Delta s. \quad (4.38)$$

The three terms appearing in this expression have a clear physical interpretation. The first contribution is positive and corresponds to the increase in local scattering when the air density increases. The two remaining contributions are negative and arise from enhanced extinction along the solar and observer optical paths. Increasing the air density therefore simultaneously increases the probability of scattering and the attenuation of photons propagating through the atmosphere.

The line integrals appearing in the weighting functions are evaluated using the same analytical formalism as that employed previously for the calculation of optical thickness (see Section 3.5). In this case, however, the extinction coefficient is replaced by the basis function $\mathcal{R}_j$.

An important advantage of the analytic formulation is that many of the quantities required for Jacobian computation are already evaluated during the radiance calculation itself. The radiance and the associated weighting functions can therefore be computed simultaneously, considerably reducing the overall computational cost. In addition, compared with perturbation methods, the analytic approach avoids a large number of unnecessary calculations.

To illustrate the structure of the Jacobian matrix, the weighting functions are shown in Figures 4.5, 4.6, and 4.7, at wavelengths of 310 nm, 350 nm, and 600 nm, as a function of altitude, for different tangent altitudes h_T . The width of the weighting functions provides insight into the vertical resolution of the measurement: the narrower the weighting function, the finer the vertical sensitivity of the retrieval.

Since the Jacobian describes the sensitivity of the measured radiances to perturbations in the logarithm of the air number density, the regions where the weighting functions reach their maximum correspond to the atmospheric layers that contribute most strongly to the observed signal. As expected, these sensitivity peaks are located close to the tangent altitude, which is consistent with the limb-scattering geometry.

Differences between wavelengths are also visible. The position and shape of the weighting functions vary with wavelength as a consequence of the wavelength dependence of Rayleigh scattering ($\propto \lambda^{-4}$). In particular, the weighting-function peaks are found at lower altitudes for 600 nm than for 310 nm and 350 nm.

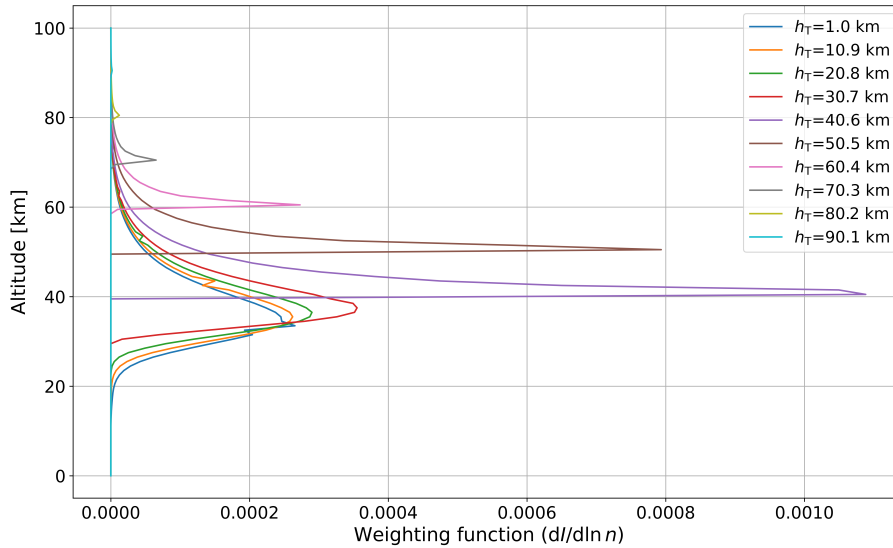


Figure 4.5: Weighting functions at $\lambda = 310$ nm for different tangent altitudes.

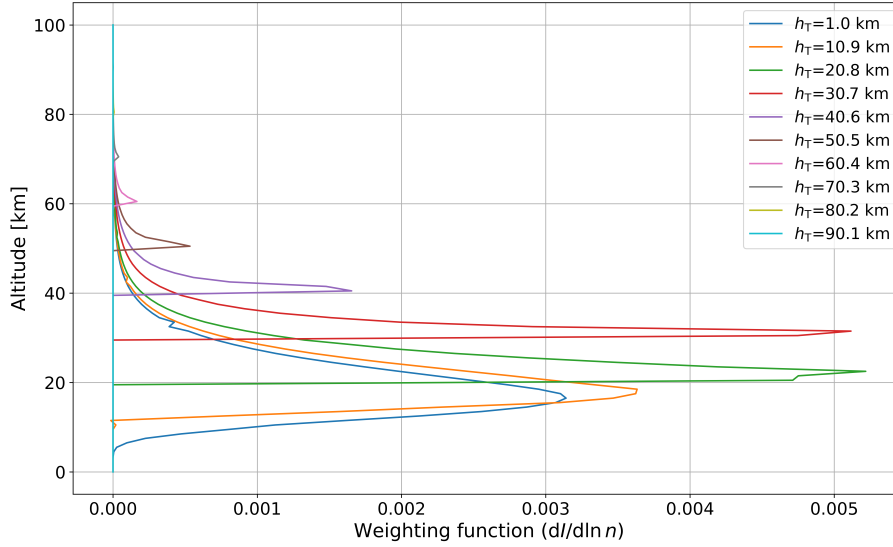


Figure 4.6: Weighting functions at $\lambda = 350$ nm for different tangent altitudes.

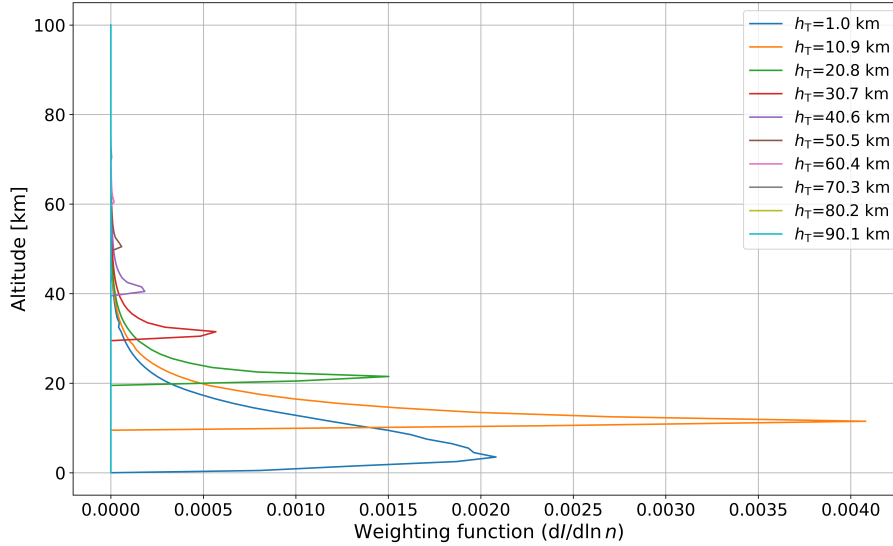


Figure 4.7: Weighting functions at $\lambda = 600$ nm for different tangent altitudes.

4.4 End-to-end temperature retrieval from radiance measurements

Having established the retrieval of air number density from radiance measurements and the derivation of temperature from air number density profiles, both steps can be combined to estimate temperature directly from limb-scattered radiances.

A synthetic radiance profile representative of observations from a limb-viewing instrument such as OMPS-LP is first generated. The SASKTRAN model is used to compute a multiple-scattered radiance profile (see Subsection 3.6.5), providing a realistic representation of the measured signal. Indeed, a limb-viewing instrument detects all photons reaching the LOS, regardless of the number of scattering events undergone before reaching the detector.

Instrumental Gaussian noise is subsequently added to the simulated radiances in order to imitate measurement uncertainties. The noise level is specified through a standard deviation defined for each radiance value as

$$S_i = \frac{y_i}{\text{SNR}_i}, \quad (4.39)$$

where y_i represents the simulated radiance at tangent altitude i , and SNR_i is the corresponding signal-to-noise ratio (SNR). An altitude-dependent SNR profile derived from OMPS-LP observations is prescribed in order to reproduce realistic observational conditions, including the degradation of measurement quality at higher altitudes. Since the SNR profile depends on wavelength, different noise levels are obtained for the two retrieval channels.

From these artificial noisy radiances, the retrieval scheme explained previously in Section 4.3 is applied to estimate the logarithm of the air number density profile. The first guess $\mathbf{x}_0$ is obtained from the mean of a set of profiles generated by the BASCOE model [51]. As a consequence, it is significantly smoother than individual atmospheric profiles. The retrieved density profile is then used to infer the corresponding atmospheric temperature profile, as described in Section 4.2. The remaining step consists in selecting the input parameters.

Default input parameters are used throughout this study (see Subsection 3.6.2). The analysis is restricted to the middle atmosphere, and only results between 35 km and 100 km are presented. The upper limit is expected to be refined in future work. The lower bound at 35 km is chosen to avoid contamination from stratospheric sulfate aerosols.

Retrievals are performed at two wavelengths, 310 nm and 350 nm, following an approach similar to Zawada et al. [15]. As discussed in Chapter 3, the radiative behavior differs significantly between these wavelengths. At 310 nm, ozone absorption becomes increasingly significant below approximately 65 km [16]. As a consequence, the 350 nm channel is expected to perform better in the lower part of the altitude range of interest (35–100 km), despite a stronger contribution from multiple scattering at this wavelength [29]. Retrievals at higher wavelengths ($\lambda > 650$ nm) are not considered, as strong aerosol scattering contamination significantly degrades the quality of the measured signal [16].

The inversion is applied to noisy radiance profiles simulated using a multiple-scattering forward model (SASKTRAN), whereas the retrieval model is based on a single-scattering approximation. Although this may appear inconsistent, the approach can be justified under specific conditions. As discussed by Zawada et al. [15], a multiplicative scaling of the radiance profile can directly translate into a scaling of the retrieved number density profile, provided that (a) the fraction of multiple scattering remains approximately constant with altitude, and (b) the optical depth along the LOS is sufficiently small for the Beer–Lambert attenuation to remain in the linear regime. Since temperature retrievals depend primarily on density gradients, such multiplicative scaling does not directly affect the retrieved temperature profile. These conditions are generally satisfied at higher altitudes in the atmosphere, as pointed out by Sheese et al. [16].

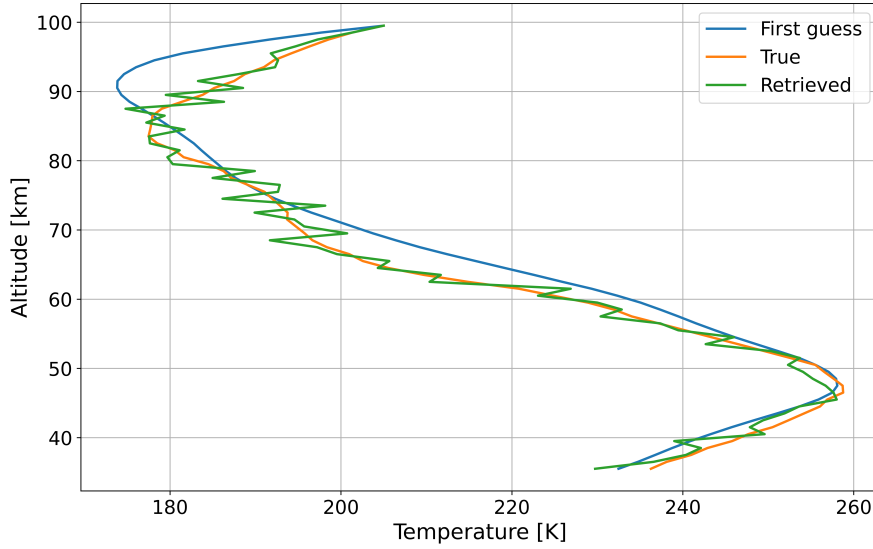


Figure 4.8: Retrieved atmospheric temperature profiles at 310 nm. The *true* profile corresponding to a perfect density retrieval (orange line), the *first-guess* profile derived from the initial state $\mathbf{x}_0$ (blue line), and the final *retrieved* profile (green line) obtained using the inversion scheme are shown.

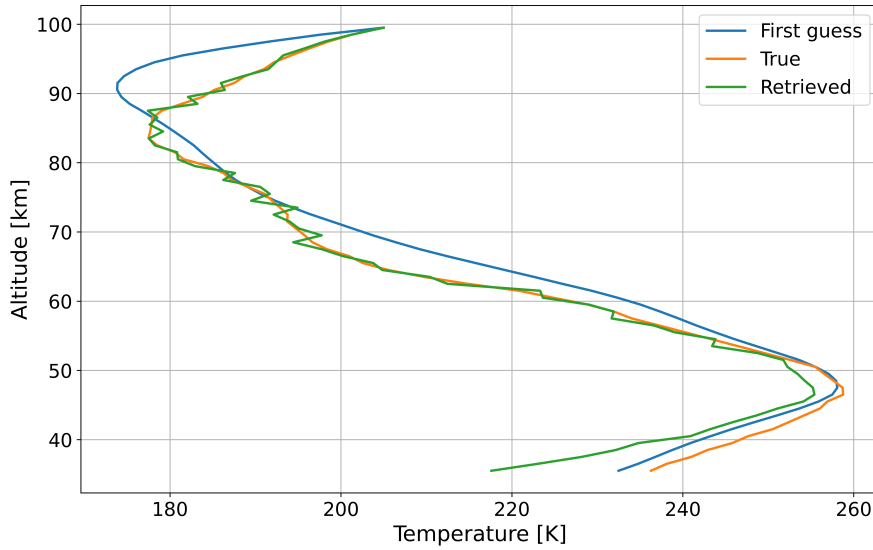


Figure 4.9: Retrieved atmospheric temperature profiles at 350 nm. The *true* profile corresponding to a perfect density retrieval (orange line), the *first-guess* profile derived from the initial state $\mathbf{x}_0$ (blue line), and the final *retrieved* profile (green line) obtained using the inversion scheme are shown.

Under these assumptions, the retrieval results are now examined. Figures 4.8 and 4.9 show the temperature profiles obtained at 310 nm and 350 nm, respectively. Three curves are displayed: (i) the *true* profile, corresponding to the temperature that would be obtained from a perfect retrieval of the air density (noting that this profile differs slightly from the true temperature profile used in SASKTRAN to generate the radiances; see Subsection 4.2.3), (ii) the *first guess* profile, derived from the initial state $\mathbf{x}_0$, and (iii) the *retrieved* profile, obtained after application of the full retrieval algorithm.

A striking feature is the presence of oscillations throughout the retrieved profile. Although the overall structure is captured, the algorithm does not fully reproduce the smoothness of the *true* profile and instead exhibits oscillatory behavior around it. These oscillations are found to be slightly less pronounced at 310 nm than at 350 nm, which is attributed to the different Gaussian noise levels applied at each wavelength. This behavior motivates the introduction of the final components of the retrieval framework, namely the inclusion of an error covariance matrix and the application of regularization techniques.

4.4.1 Regularized least squares solution with errors

To improve the temperature retrievals, the *measurement error covariance matrix*, denoted by $\mathbf{S}_\varepsilon$, is first introduced into the retrieval framework. Indeed, every measurement is affected by uncertainties arising from various sources, including instrumental noise, calibration inaccuracies, and modeling approximations. These uncertainties are commonly represented by an additive error term ε , which is assumed to follow a *multivariate centered* (with zero mean) *Gaussian distribution*,

$$\varepsilon \in \mathbb{R}^m \sim \mathcal{N}(\mathbf{0}, \mathbf{S}_\varepsilon). \quad (4.40)$$

The associated covariance matrix,

$$\mathbf{S}_\varepsilon = \mathbb{E} [\varepsilon \varepsilon^T] \in \mathbb{R}^{m \times m}, \quad (4.41)$$

quantifies the uncertainty of the measurements, where $\mathbb{E}[\cdot]$ denotes the expected value operator. The diagonal elements correspond to the variances of the individual measurements, while the off-diagonal elements describe possible correlations between measurement errors.

Although measurement errors are generally correlated to some extent, it is assumed here that radiance measurements performed at different tangent altitudes are statistically independent. Under this assumption, $\mathbf{S}_\varepsilon$ becomes diagonal, which considerably simplifies its inversion [58]. It can therefore be written as

$$\mathbf{S}_\varepsilon = \text{diag} (S_1^2, \dots, S_m^2), \quad (4.42)$$

where S_i is given by Equation (4.39).

The cost function is therefore modified to account for the measurement uncertainties and becomes

$$\mathcal{J}(\mathbf{x}) = \|\mathbf{y} - \mathbf{F}(\mathbf{x})\|_{\mathbf{S}_\varepsilon^{-1}}^2 = (\mathbf{y} - \mathbf{F}(\mathbf{x}))^T \mathbf{S}_\varepsilon^{-1} (\mathbf{y} - \mathbf{F}(\mathbf{x})). \quad (4.43)$$

Applying this weighted least squares formulation within the framework of the Levenberg–Marquardt algorithm yields

$$\hat{\mathbf{x}}^{(i+1)} = \hat{\mathbf{x}}^{(i)} + \left(\mathbf{K}^{(i)T} \mathbf{S}_\varepsilon^{-1} \mathbf{K}^{(i)} + \gamma^{(i)} \text{diag} \left(\mathbf{K}^{(i)T} \mathbf{S}_\varepsilon^{-1} \mathbf{K}^{(i)} \right) \right)^{-1} \mathbf{K}^{(i)T} \mathbf{S}_\varepsilon^{-1} (\mathbf{y} - \mathbf{F}(\hat{\mathbf{x}}^{(i)})). \quad (4.44)$$

As observed previously, measurement noise introduces oscillatory structures into the retrieved temperature profiles. To mitigate this effect, an additional constraint is imposed through *Tikhonov regularization* [59]. The retrieval problem is then formulated as the minimization of

$$\begin{aligned}\mathcal{J}(\mathbf{x}) &= \|\mathbf{y} - \mathbf{F}(\mathbf{x})\|_{\mathbf{S}_\epsilon^{-1}}^2 + \beta \|\mathbf{\Gamma}(\mathbf{x} - \mathbf{x}_0)\|^2 \\ &= (\mathbf{y} - \mathbf{F}(\mathbf{x}))^T \mathbf{S}_\epsilon^{-1} (\mathbf{y} - \mathbf{F}(\mathbf{x})) + \beta (\mathbf{x} - \mathbf{x}_0)^T \mathbf{\Gamma}^T \mathbf{\Gamma} (\mathbf{x} - \mathbf{x}_0),\end{aligned}\quad (4.45)$$

where $\mathbf{\Gamma}$ denotes the *Tikhonov regularization matrix* and β is the *regularization parameter*. This additional constraint incorporates prior information into the inversion and establishes a compromise between fitting the forward model to the measurements and maintaining a smooth retrieved state [31]. The regularization parameter β controls the strength of the constraint. Larger values promote smoother solutions by suppressing oscillations caused by measurement noise. However, excessively large values may over-constrain the retrieval, causing the solution to remain excessively close to the initial first guess and reducing the contribution of the measurements.

Several forms of Tikhonov regularization exist. Here, *second-order Tikhonov regularization* is employed. The corresponding regularization matrix is defined as the *discrete second-derivative operator* [60],

$$\mathbf{\Gamma} = \mathbf{L}_2 = \begin{pmatrix} 1 & -2 & 1 & 0 & \cdots & 0 \\ 0 & 1 & -2 & 1 & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & 1 & -2 & 1 \end{pmatrix} \in \mathbb{R}^{(n-2) \times n} \quad (4.46)$$

The second-derivative operator constrains the shape of the retrieved profile and specifically penalizes large second derivatives, i.e., excessive curvature or roughness in the solution.

Combining the error covariance matrix, the second-order Tikhonov regularization, and the Levenberg–Marquardt damping term finally leads to the retrieval update equation

$$\begin{aligned}\hat{\mathbf{x}}^{(i+1)} &= \hat{\mathbf{x}}^{(i)} + \left(\mathbf{K}^{(i)T} \mathbf{S}_\epsilon^{-1} \mathbf{K}^{(i)} + \beta \mathbf{L}_2^T \mathbf{L}_2 + \gamma^{(i)} \text{diag} \left(\mathbf{K}^{(i)T} \mathbf{S}_\epsilon^{-1} \mathbf{K}^{(i)} \right) \right)^{-1} \\ &\quad \times \left[\mathbf{K}^{(i)T} \mathbf{S}_\epsilon^{-1} (\mathbf{y} - \mathbf{F}(\hat{\mathbf{x}}^{(i)})) - \beta \mathbf{L}_2^T \mathbf{L}_2 (\hat{\mathbf{x}}^{(i)} - \mathbf{x}_0) \right].\end{aligned}\quad (4.47)$$

This expression constitutes the final retrieval algorithm used to estimate atmospheric temperature profiles from limb radiance measurements.

A remaining key aspect is the determination of the regularization parameter β . Several approaches exist to define an appropriate strength for the constraint [60]. In this work, we select β by inspecting the relative magnitude of the two terms in Equation (4.45) and tuning it through a trial-and-error approach. The value retained for the simulations presented below is $\beta = 10^5$. This relatively large value is chosen to ensure that the regularization term dominates over the contribution of the measurement error covariance term, whose inverse typically has large diagonal elements. A more systematic optimization of this parameter could nevertheless be performed.

Figures 4.10 and 4.11 show the retrieved atmospheric temperature profiles at 310 nm and 350 nm, respectively, using $\beta = 10^5$ and the measurement error covariance matrix defined above. The oscillations observed in Figures 4.8 and 4.9

are significantly reduced, resulting in smoother retrieved profiles. At 310 nm, the retrieval performs very well over the altitude range considered, with the *retrieved* profile closely following the *true* profile. At 350 nm, the retrieval remains meaningful but shows larger deviations from the *true* profile compared to the 310 nm case.

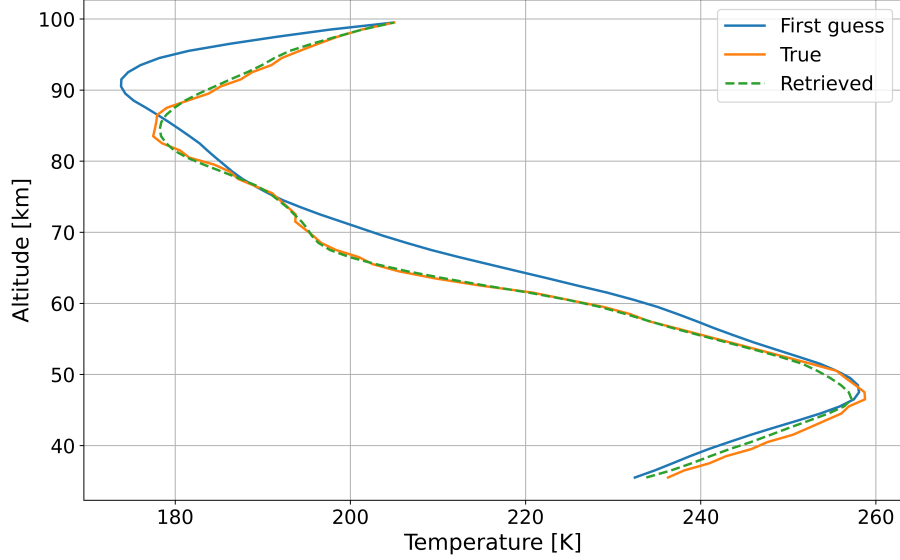


Figure 4.10: Retrieved atmospheric temperature profile at 310 nm using second-order Tikhonov regularization ($\beta = 10^5$). The *true* profile corresponding to a perfect density retrieval (orange line), the *first-guess* profile derived from the initial state $\mathbf{x}_0$ (blue line), and the final *retrieved* profile (green dashed line) obtained using the full inversion scheme are shown.

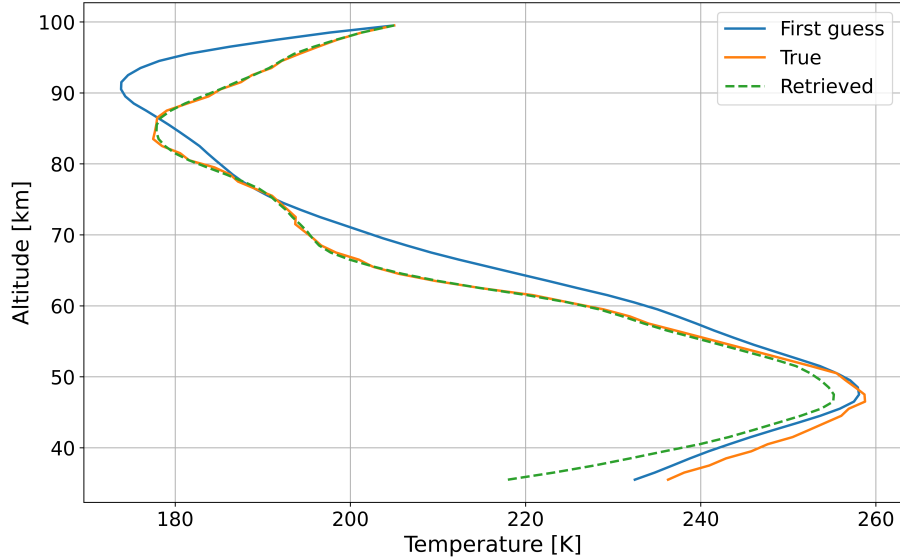


Figure 4.11: Retrieved atmospheric temperature profile at 350 nm using second-order Tikhonov regularization ($\beta = 10^5$). The *true* profile corresponding to a perfect density retrieval (orange line), the *first-guess* profile derived from the initial state $\mathbf{x}_0$ (blue line), and the final *retrieved* profile (green dashed line) obtained using the full inversion scheme are shown.

Overall, these results indicate that the retrieval algorithm is capable of accurately retrieving temperature profiles in the middle atmosphere, forming the basis for its application to real observational data.

4.4.2 Application to OMPS-LP observations

The ultimate test of the retrieval algorithm is its application to real atmospheric measurements. For this purpose, radiance observations acquired by the OMPS-LP instrument are used.

The OMPS-LP instrument is onboard the Suomi-NPP satellite, launched in 2011 into a Sun-synchronous orbit [24]. The primary objective of the OMPS mission is to provide continuous global observations of atmospheric ozone and thereby contribute to the long-term monitoring of stratospheric ozone recovery. Temperature can also be retrieved as a secondary product [17].

The limb profiler simultaneously images the full vertical extent of the atmospheric limb through three vertical slits and measures spectrally resolved radiance profiles over a broad spectral range extending from approximately 290 nm to 1000 nm, covering the UV, visible, and near-IR regions of the spectrum. The incoming radiation is dispersed by a prism before being recorded on a two-dimensional charge-coupled device (CCD) detector. Owing to its limb-viewing geometry, the instrument provides ozone profile measurements with a vertical resolution of approximately 1.5–2 km in the stratosphere [24].

The data used here originate from the Level-1 Gridded (L1G) OMPS-LP product [61]. This product provides calibrated limb radiances interpolated onto a regular wavelength–altitude grid after correction of instrumental distortions. For each observation scene, a radiance profile is available on the altitude grid defined in (3.21), making the dataset particularly suitable for the retrieval framework developed in this work.

In contrast to the synthetic simulations presented previously, where all input parameters could be prescribed freely, the only degrees of freedom available here are the observation date and the selected event, i.e., a normalized limb-scattered radiance profile at a given wavelength. Since the wavelengths provided in the OMPS-LP dataset are not uniformly spaced at 1 nm intervals, the wavelength used in the retrieval corresponds to the available channel closest to the value specified by the user.

Figures 4.12 and 4.13 present normalized radiance profiles from OMPS-LP at $\lambda = 312.93$ nm and $\lambda = 350.48$ nm, respectively. In both cases, the observed radiance profiles are shown alongside the corresponding single-scattering simulations from the present RTM and the multiple-scattering simulations generated with SASKTRAN.

Two important features can be observed. First, the OMPS-LP measurements are spatially limited, with radiance profiles not extending beyond approximately 70 km in tangent altitude. Second, the observed radiance generally follows the multiple-scattering simulations reasonably well; however, a systematic contamination is apparent. This discrepancy is commonly attributed to *stray light*, i.e. parasitic light reaching the detector when it should not. Although OMPS-LP applies correction algorithms and dedicated preprocessing steps to mitigate stray light contamination, residual effects remain in the processed data [24]. This is an instrumental effect inherent to the measurement system.

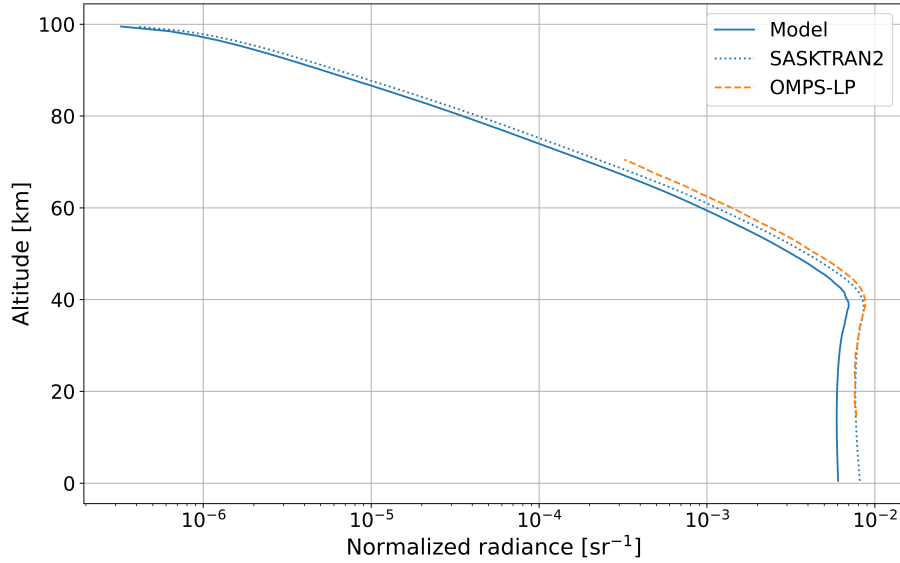


Figure 4.12: Normalized OMPS-LP limb-scattered radiance profile at $\lambda = 312.93$ nm (orange dashed line) for orbit 49 060 on 9 March 2026, shown together with single-scattering simulations from the present RTM (blue solid line) and multiple-scattering calculations from SASKTRAN (blue dotted line).

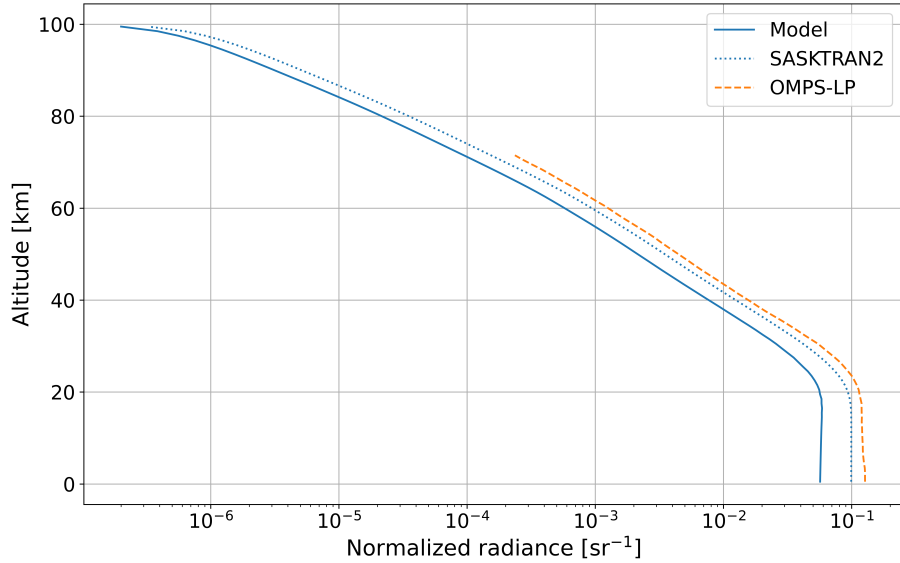


Figure 4.13: Normalized OMPS-LP limb-scattered radiance profile at $\lambda = 350.48$ nm (orange dashed line) for orbit 49 060 on 9 March 2026, shown together with single-scattering simulations from the present RTM (blue solid line) and multiple-scattering calculations from SASKTRAN (blue dotted line).

Another possible source of enhanced radiance is the presence of *polar mesospheric clouds* (PMCs) [16, 62]. However, PMCs occur only at high latitudes during the summer months, typically between 80 and 85 km altitude. Since the selected OMPS-LP profile was acquired on 9 March 2026 at low latitudes, PMC contamination is not expected to contribute significantly to the observed radiance enhancement.

We conclude this section with limited results. The Figures 4.14 and 4.15 show the *retrieved* temperature profiles together with the corresponding *first-guess* tem-

perature profiles at 310 nm and 350 nm. No definitive conclusions can be drawn from these results. Since both retrievals are based on the same observation date, the resulting temperature profiles at the two wavelengths are expected to be similar. This appears to be the case; however, no external validation is available, for instance through an independent retrieval performed by another study. As a result, this section remains inconclusive.

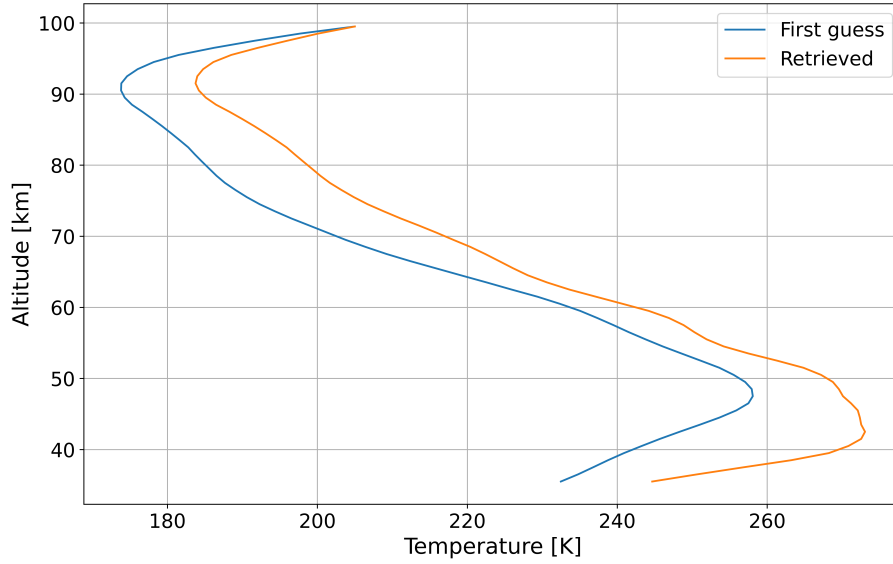


Figure 4.14: Retrieved atmospheric temperature profile at 312.93 nm applied to OMPS-LP data for orbit 49 060 on 9 March 2026. The *first-guess* profile derived from the initial state $\mathbf{x}_0$ (blue line) and the final *retrieved* profile (orange line) obtained from the full inversion scheme are shown.

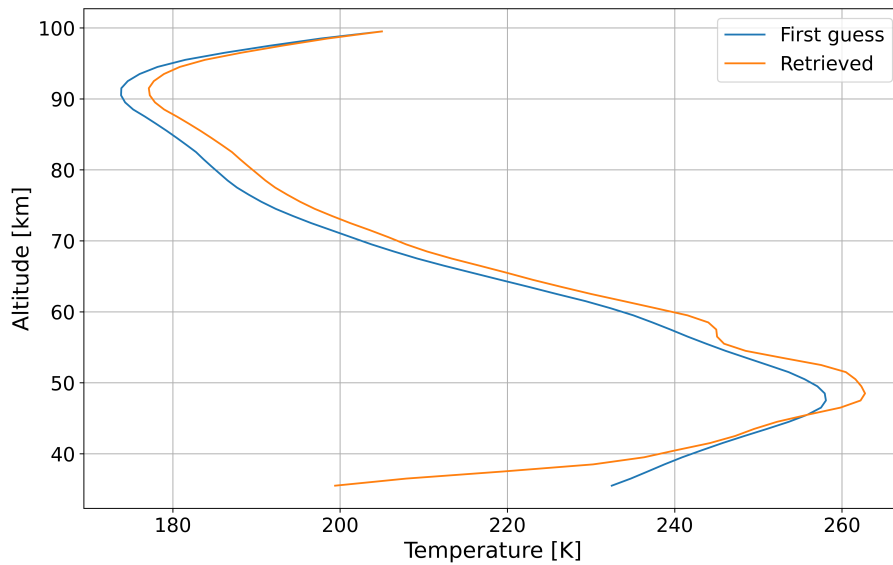


Figure 4.15: Retrieved atmospheric temperature profile at 350.48 nm applied to OMPS-LP data for orbit 49 060 on 9 March 2026. The *first-guess* profile derived from the initial state $\mathbf{x}_0$ (blue line) and the final *retrieved* profile (orange line) obtained from the full inversion scheme are shown.

Chapter 5

Conclusions and outlook

During this Master’s thesis, a 1D spherical scalar RTM based on the single-scattering approximation was fully implemented in Python. The objective of this model is to simulate radiance profiles for a given atmospheric state, including atmospheric constituent concentrations as well as thermodynamic parameters such as temperature and pressure. Only Rayleigh scattering and ozone absorption were considered, a choice justified by the focus on the middle atmosphere. The model was subsequently compared and validated against the reference SASKTRAN model, showing relative radiance differences below 1% for all tangent altitudes and for the three selected wavelengths, namely $\lambda = 310$ nm, 350 nm, and 600 nm.

This development is particularly relevant in the context of the upcoming ALTIUS mission. The code will be transferred to the ALTIUS team, providing a simple Belgian forward model that can be used for the bright limb observation mode of the instrument [25] (see Figure 5.1). Despite several delays in the satellite’s launch, the current expected launch year is 2027.

As part of ESA’s Earth Watch programme, ALTIUS is expected to provide the atmospheric science community with an unprecedented view of the temporal and spatial evolution of ozone and related trace gases. In this context, the preparation of reliable forward and inverse modeling tools prior to launch is essential to ensure that, once the first measurements become available, retrievals of ozone (the primary product), other atmospheric constituents, and temperature (secondary products) can be performed in an operational manner.



Figure 5.1: Artistic view of ALTIUS observing the Earth atmospheric limb (from [63]).

The second part of this work focused on one application of the model, namely the retrieval of temperature profiles in the middle atmosphere. The forward model was therefore used as the basis for an inverse problem, i.e. the retrieval of the atmospheric state from radiance measurements. This process was carried out in two main steps: (i) estimation of (the logarithm of) the air number density from radiance profiles, and (ii) retrieval of the temperature profile from the retrieved density using hydrostatic equilibrium combined with the ideal gas law. The first step was performed using a Levenberg–Marquardt algorithm with second-order Tikhonov regularization, through Equation (4.47). Temperature retrievals were performed at 310 nm and 350 nm using synthetic radiance data generated with the SASKTRAN model.

The results are encouraging, particularly at 310 nm, although the analysis remains primarily qualitative. A more rigorous quantitative assessment would require the application of the formalism of Rodgers [55], which provides diagnostic tools such as the retrieval error covariance matrix and the averaging kernel, allowing a more complete characterization of the sensitivity of the solution to the true atmospheric state. In addition, Sheese et al. [16] combined information from two wavelengths, thereby improving retrieval quality, as different spectral regions provide complementary sensitivity to different altitude ranges.

Finally, the application of the full inversion chain to real OMPS-LP observations was only partially completed. At this stage, no definitive conclusions can be drawn from this incomplete analysis. A more conclusive assessment would require systematic validation against independent retrievals derived from OMPS-LP data or from other satellite instruments. More broadly, a complete analysis of the long-term OMPS-LP record (2012–present) would make it possible to investigate whether previously observed stratospheric cooling trends persist.

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