



UNIVERSIDAD DE LA REPÚBLICA
FACULTAD DE INGENIERÍA



Solar Spectral Irradiance Modelling and Retrieval of Aerosol Optical Depth from Ground Measurements

TESIS PRESENTADA A LA FACULTAD DE INGENIERÍA DE LA UNIVERSIDAD
DE LA REPÚBLICA POR

Paola Russo Ganón

EN CUMPLIMIENTO PARCIAL DE LOS REQUERIMIENTOS
PARA LA OBTENCIÓN DEL TÍTULO DE
MASTER EN INGENIERÍA DE LA ENERGÍA.

DIRECTORES DE TESIS

Gonzalo Abal Guerault Universidad de la República
Agustín Laguarda Cirigliano Universidad de la República

TRIBUNAL

Rodrigo Alonso Suárez Universidad de la República
Fernando Ramos Martins Universidade Federal de São Paulo
Javier Pereyra Universidad de la República

DIRECTOR ACADÉMICO

Gonzalo Abal Guerault Universidad de la República

Montevideo
lunes 6 julio, 2026

Solar Spectral Irradiance Modelling and Retrieval of Aerosol Optical Depth from Ground Measurements, Paola Russo Ganón.

ISSN 1688-2806

Esta tesis fue preparada en L^AT_EX usando la clase iietesis (v1.1).

Contiene un total de 183 páginas.

Compilada el lunes 6 julio, 2026.

<http://iie.fing.edu.uy/>

*Dedicated to the memory of my beloved father
Rodney.*

*Thank you for being there every day with the
love and guidance I needed.*

I will always remember you.

Acknowledgements

First of all, I would like to express my profound gratitude to my supervisors, Dr. Gonzalo Abal and Dr. Agustín Laguarda, for having honoured me with the opportunity to pursue my MSc. studies under their supervision and to work on these interesting topics at the Solar Energy Laboratory. Their valuable insights and contributions helped me grow both academically and personally, and I hope to have met their expectations.

I am sincerely grateful to Dr. José Cataldo, Director of SCAPA, for his continuous support throughout my Master's studies. I extend the thanks to all the members of SCAPA, who followed the advances of the thesis, and the secretaries Teresa and Diana, for their excellent administrative assistance.

I am much obliged to the members of the thesis evaluation committee: Dr. Rodrigo Alonso, Dr. Fernando Martins, and Dr. Javier Pereyra, who kindly agreed to review this work.

I am thankful to the institutions: Universidad de la República, Uruguay (UdelaR), the Engineering Faculty (FING), CENUR Litoral Norte, the Physics Department (DFL) and the Solar Energy Laboratory (LES). To all my work colleagues, among them, Dir. Dr. Rodrigo Alonso, Mag. José Di Laccio, Mag. Gerardo Vitale, Dr. Italo Bove, Dr. Juan Rodríguez, Mag. Inti Piccioli, Ing. Liber Dovat, Andrés Monetta, for having provided an excellent work environment.

I gratefully acknowledge the financial support received from Agencia Nacional de Investigación e Innovación (ANII), the Master's scholarship awarded was of essential importance.

I am deeply grateful to all my scientist friends around the world, whom I had the privilege of meeting throughout this journey; specially Dr. Lionel Doppler, Dr. Stefan Wacker, Dr. Francisco Navas, Dr. Philip Blanc, Dr. Yves-Marie Saint-Drenan, Dr. Benoît Gschwind, Dr. Stephen Volz and Dr. Diego Pavanello. They enlightened me with their knowledge and kindness, and made the culmination of this research possible.

I express my deepest thanks to my admired friend, Philip Hanham, who helped me nurture my English language. None of my interactions in English, books read or manuscripts written, would have ever taken place, without the knowledge and advice he has given me.

Last but not least, thank you ever so much to my family, who have always been there for me: my amazing mum Perla, my extraordinary sister Stephanie, and my lovely niece and nephew, Cami and Maxi.

Summary

Accurate modelling and monitoring of solar irradiance is essential for advancing solar energy applications, atmospheric research, and broader environmental studies. This thesis addresses three complementary aspects of solar irradiance and its interaction with the atmosphere in Uruguay. First, the occurrence of over-irradiance events (OIE) is statistically characterized for the first time in the country, quantifying their frequency, duration, and intensity throughout the seasons. Second, the performance of two widely used physical clear-sky models, SMARTS (spectral) and REST2 (broadband), is assessed against high-resolution ground measurements, evaluating the influence of input atmospheric parameters and data sources. Third, a retrieval methodology for aerosol optical depth (AOD) is implemented using measurements from a collimated spectroradiometer (EKO MS-711), and validated against independent AERONET observations. The results demonstrate that OIE are a non negligible phenomenon in Uruguay, that clear-sky models can reproduce local conditions with good accuracy when provided with appropriate atmospheric inputs, and that reliable AOD retrievals can be obtained from accessible instrumentation. Overall, this work contributes new knowledge on physical solar irradiance modelling in Uruguay, providing tools and methodologies relevant for renewable energy deployment, atmospheric monitoring, and environmental applications.

Resumen

Modelar y monitorear la irradiancia solar con precisión es fundamental para el avance de las aplicaciones de energía solar, la investigación atmosférica y los estudios ambientales en general. Esta tesis aborda tres aspectos complementarios de la irradiancia solar y su interacción con la atmósfera en Uruguay. En primer lugar, se caracteriza estadísticamente, por primera vez en el país, la ocurrencia de eventos de sobre-irradiancia (OIE), cuantificando su frecuencia, duración e intensidad a lo largo de las distintas estaciones del año. En segundo lugar, se evalúa el desempeño de dos modelos físicos de cielo claro ampliamente utilizados, SMARTS (espectral) y REST2 (de banda ancha), frente a mediciones terrestres de alta resolución temporal, analizando la influencia de los parámetros atmosféricos de entrada y de las fuentes de datos empleadas. En tercer lugar, se implementa una metodología de estimación de la profundidad óptica de aerosoles (AOD) utilizando mediciones provenientes de un espectrorradiómetro colimado (EKO MS-711), la cual se valida mediante estimativos independientes de la red AERONET. Los resultados demuestran que los OIE constituyen un fenómeno no despreciable en Uruguay, que los modelos de cielo claro pueden reproducir adecuadamente las condiciones locales cuando se emplean parámetros atmosféricos apropiados, y que es posible obtener estimaciones confiables de AOD a partir de instrumentación accesible. En conjunto, este trabajo aporta nuevo conocimiento sobre el modelado físico de la irradiancia solar en Uruguay, proporcionando herramientas y metodologías de relevancia para el desarrollo de las energías renovables, el monitoreo atmosférico y las aplicaciones ambientales.

Contents

Summary

Resumen

1. Introduction	1
1.1. Background and motivation	1
1.2. Objectives	4
1.3. Organization of this thesis	5
2. Solar Radiation in the Atmosphere	6
2.1. Fundamental concepts of solar radiation	6
2.2. Solar radiation in the atmosphere	11
2.3. Over-irradiance or cloud enhancement	21
2.4. Surface and atmospheric information	22
2.5. Performance metrics	32
3. Statistical analysis of over-irradiance events in Uruguay	35
3.1. Methodology	35
3.1.1. Data	35
3.1.2. Over-irradiance detection	36
3.2. Statistical characterization of OIE	39
3.3. Conclusions	45
4. SMARTS clear-sky spectral irradiance model	47
4.1. SMARTS description	48
4.1.1. Beam spectral irradiance	51
4.1.2. Diffuse spectral irradiance	58
4.1.3. SMARTS outputs	61
4.1.4. Previous assessments	62
4.2. Methodology	66

4.2.1. Broadband and spectral irradiance ground measurements	66
4.2.2. Different atmospheric inputs tested with SMARTS	70
4.3. Results	74
4.3.1. Sensitivity of SMARTS to relevant input parameters	74
4.3.2. Performance of SMARTS spectral estimates	77
4.3.3. Performance of SMARTS broadband irradiances	85
4.4. Conclusions	89
5. Assessment of the clear-sky broadband irradiance model REST2	90
5.1. Model overview	91
5.1.1. Beam normal irradiance	91
5.1.2. Diffuse and global horizontal irradiance	92
5.1.3. Previous validations for REST2	94
5.2. Data and methods	95
5.2.1. Ground measurements of solar irradiance	95
5.2.2. Atmospheric information	95
5.2.3. Quality control and clear-sky selection	97
5.3. Performance of REST2 model	99
5.4. Conclusions	102
6. Retrieval of Aerosol Optical Depth from spectral irradiance ground measurements	103
6.1. Methodology	104
6.1.1. Inversion Algorithm	105
6.1.2. Circumsolar Correction	108
6.1.3. TOA Spectral Irradiance	108
6.2. Results	111
6.3. Conclusions	116
7. Closing remarks	118
Glossary	I
A. Appendix: Measurement instruments	VI
A.1. EKO spectroradiometer technical description	VI
A.2. Spectroradiometer traceability	VIII
A.3. Broadband traceability	VIII
B. Appendix: additional theoretical details	X
B.1. Sun-Earth distance correction factor, F_n	X
B.2. Air masses related to different atmospheric processes	X
B.3. Air masses used specifically in REST2	XI
B.4. Downward fraction of scattered radiation, F_R	XI

B.5.	Effective ozone transmittance, $\Gamma_{0\lambda}$	XII
B.6.	Single scattering albedo and aerosol asymmetry parameter	XII
B.7.	Single Scattering Albedo from Braslau & Dave	XIII
B.8.	Back scattering infinite inter reflections	XIII
B.9.	Parametrization coefficients for the air masses, SMARTS	XV
B.10.	Reference atmosphere values for STS and STW in SMARTS	XV
B.11.	Transmittance computation	XVI
B.12.	Aerosol model (Shettle & Fenn) for obtaining α_1 and α_2 depending on the relative humidity in SMARTS	XVII
B.13.	Full Width at Half Maximum (FWHM)	XVIII
B.14.	PAR conversion ratio from photon flux to irradiance	XIX
C.	Appendix: Additional results	XXI
C.1.	Statistics of atmospheric parameters	XXI
C.2.	Statistics of atmospheric parameters used in SMARTS smoothed	XXIII
C.3.	Statistics of atmospheric parameters used in SMARTS raw	XXIV
C.4.	Estimated spectroradiometer uncertainty	XXVI
C.5.	Broadband performance of SMARTS for a single day	XXIX

List of Tables

List of Figures

Chapter 1

Introduction

1.1. Background and motivation

As a signatory nation of the Paris agreement (United Nations, 2015), Uruguay has been engaged in contributing to the sustainable development goals, from improvements in the energy generation industry to new alternatives in agricultural production practices or energy efficiency in buildings. This has been accomplished with the support of research lines that helped develop the country technologically in these areas. Nowadays, Uruguay is known for having an electric energy matrix composed of 97 % renewable sources, in average (ADME, 2022; UruguayXXI, 2022). During the 1930s-1980s, when there was a worldwide boom to explore the exploitation limits of water resources to generate energy, several high profile hydraulic power projects were implemented in Uruguay, and are still active to this day (Caffaro, 2020; Salto Grande, 1997; Waiter, 2019). In the context of the integration of fluctuating renewable sources (wind and solar) these hydroelectric projects have provided the essential buffer, e.g. operational demand following capabilities, which helps stabilize the whole country generation park, including a high share of non-conventional renewable sources (wind and solar). In 2015, wind power farms started to operate, supported by large investor companies that came to the country attracted by convenient long term deals for the energy produced. Around the same time, photovoltaic energy benefited from a fast price drop in PV panels that allowed it to become economically competitive to be installed in small and medium size generation farms (Alberdi and Artigas, 2010; PresidenciaUy, 2013). Additionally, since 2007, biomass has become an important contributor to the energy matrix, mainly due to the establishment of cellulose pulp industries that use their production wastes for energy generation. Nowadays, the latest projects underway are related green hydrogen generation for export, made from renewable energy surplus (UruguayXXI, 2023). The current electrical generation matrix is comparable to that of Denmark, Ireland or Portugal, which is good considering Uruguay is a developing country. Of course, there is plenty of room for improvement, for example in the transport industry, where the source of energy and emissions still needs to be changed. However this is known to be one of the most challenging transitions even in any country.

In the middle of this timeline, the Solar Energy Laboratory (LES) from Universidad de la

República (<http://les.edu.uy/>), formally founded in 2015, emerges as an important actor in the appropriation and generation of scientific knowledge about solar energy. Among its early research results, the following is highlighted: the first and second Solar Maps of Uruguay in (Abal et al., 2010; Alonso-Suárez et al., 2014), the generation of a Typical Meteorological Year (TMY, known in Uruguay as AMTUes) (Alonso-Suárez et al., 2012), a server platform for satellite images reception and processing, and the installation of a ground measurement network of 8 permanent sites, which now has more than 10 years of continuous measurements of controlled quality solar irradiance recorded at 1-minute intervals. Additionally, several scientific articles and research related to the solar resource and innovative solar energy applications have been produced by LES¹. LES also offers a pyranometer calibration service aimed to support the traceability and reliability of ground measurements used in photovoltaic power plants and research centres in the country. This service implements the international standards (ISO 17025:2017, 2017; ISO 9847:2023(E), 2023). Moreover, solar consulting services are provided upon request.

The first solar irradiance models approached by the laboratory were empirical satellite all-sky models (Alonso-Suárez et al., 2012). Later, empirical clear-sky models were studied (Laguarda and Abal, 2019; Laguarda et al., 2020). Aiming to expand the measurement capabilities and to advance in the research of physical solar irradiance models, in 2020 the laboratory acquired a new spectroradiometer for measuring direct normal spectral irradiance, followed in 2022 by the acquisition of a spectroradiometer to measure global spectral irradiance. The scientific question intended to answer was: can physical models be used as a basis to reliably estimate solar spectral irradiance in the region of Uruguay? This leads to some important questions addressed in this thesis, such as: is the available atmospheric information accurate enough for a reliable physical modelling?.

The interest in physical models resides in the fact that they offer a wide range of physical information, and their possibilities go beyond the estimation of solar broadband irradiance. They can be used to estimate irradiance at different spectral bands, such as Ultraviolet (UV, 280–400 nm), Photosynthetically Active Radiation or Visible (PAR or VIS, 400–700 nm), and Near Infrared (NIR, 700–1100 nm), as well as specific atmospheric parameters (such as ozone, water vapour or aerosol concentrations, as shown in Chapter 6 of this work). Furthermore, they also allow to determine ground level irradiance with high spectral resolution (e.g. 1 nm). The accurate modelling of solar spectral irradiance is important because different spectral ranges directly govern key processes related to our everyday lives, other living beings and the whole environment. In particular, the UV range is fundamental for assessing biological effects on human and animal health, such as skin melanoma risks and ocular health (Bernhard et al., 1997; Möttus et al., 2011). It is also important for the study of degradation of materials (Shamachurn and Betts, 2016) and at LES there is a specific research line on UV irradiance (Laguarda and Abal, 2019; Laguarda et al., 2024). The PAR range is a critical driver of photosynthesis and thus central to improve agricultural productivity, estimate crop yields, or improve crop quality, both

¹See <http://les.edu.uy/investigacion/publicaciones-cientificas/> for a publication list.

in extensive agriculture and in greenhouses (Atsushi, 2016; DiLaccio et al., 2024; Habyarimana et al., 2019). Precise solar spectral knowledge is also required for technological applications in solar energy, where it is essential for the design and efficiency optimization of photovoltaic (PV) power plants due to the spectral selectivity of the PV modules (Nann and Emery, 1992). It is crucial in the development of efficient and durable materials for concentrated solar power (Kaluba et al., 2016). Furthermore, it is also required for building efficiency and comfort, for instance, in the design of smart windows that balance light harvesting and thermal comfort in buildings (Meng et al., 2022). For the relevance exposed, Chapter 4 is dedicated to the study of the spectral irradiance model SMARTS.

Due to all this applications, clouds are an undeniably important factor in the atmospheric interactions with radiation. When they occur, most of the times they attenuate radiation, meaning less radiation reaches the ground surface than the amount that reached the top of the atmosphere. However, sometimes they forward scatter and reflect light near the Sun-Earth direction, creating a magnifying glass effect, producing a short-lived phenomenon called over irradiance (or cloud enhancement of solar radiation), which implies a higher contribution from the diffuse component and ultimately that more irradiance reaches the ground than would otherwise. To take into account this relevant phenomenon, Chapter 3 of this work provides the first study of the statistical characteristics of over-irradiance events (OIE) in Uruguay.

There are two main categories of physical models for estimating ground level solar irradiance: clear-sky and all-sky models. Clear-sky models do not consider the effects of clouds on radiation, whilst all-sky model do. Clouds are dynamic and highly variable, and their effects on solar radiation are difficult to model with precision. This is because they can be located in different atmospheric layers, their inner composition can be of different types, their density can be stratified with the height and there can be variable amounts of droplets, water vapour, ice crystals, dissolved compounds and suspended particles present in the cloud (Pruppacher and Klett, 1997). For these reasons, several modern all-sky models use a combination of a clear-sky model plus satellite information, to describe cloud type, location and impact on irradiance at a given location. For example, Cloud Index Models (CIM), such as SUNY (Perez et al., 2002) and LCIM (Laguarda et al., 2020), use the irradiance under clear-sky conditions, $G_{h,cs}$, by a clear-sky model and an attenuation factor obtained from satellite information, to estimate all-sky conditions. On another modern approach, the Physical Solar Model (PSM) (Habte et al., 2017), uses the calculated irradiance for clear-sky conditions, estimated in this case with the clear-sky model REST2 (Gueymard, 2008b), and separately, a physically modelled irradiance for cloudy conditions. Since clear-sky models play a fundamental role in several approaches to estimate all-sky conditions, in Chapter 4 (spectral model SMARTS) and Chapter 5 (broadband model REST2) a performance analysis of clear-sky physical solar irradiance models is presented, as a first step to obtain all-sky conditions models.

Obtaining high quality atmospheric information is difficult, but it is essential for the physical modelling of atmospheric processes, including solar radiation absorption and scattering. It is

also important for monitoring the atmosphere, calibrating satellites, and validating reanalysis data bases. Even though nowadays there are several global sources of atmospheric information available (such as satellite-based estimates and reanalysis databases), ground stations measuring reliable atmospheric information in South America are sparsely located. An important atmospheric parameter is Aerosol Optical Depth (AOD). It is related to the concentration of aerosols in the atmosphere, which play an important role in the Earth's energy balance (Chen et al., 2010), cloud formation (Seinfeld et al., 2016), human health (Johannson et al., 2015) and atmospheric radiative processes affecting the solar irradiance reaching the ground surface (Gueymard and Ruiz-Arias, 2016). They are related to global warming, water cycles, energy production, and human health risks (Braithwaite et al., 2019; DeBont et al., 2022). Due to the characteristics of AOD, this parameter needs a fairly precise estimation, however its estimates in global reanalysis databases are not accurate enough (Laguarda and Abal, 2020). Usually, the most precise retrievals of AOD are based on measurements of well maintained Sun Photometers (Giles et al., 2019). But nowadays, the advances in commercial spectroradiometers (lower cost instruments, not specifically designed to perform these retrievals), have made them a competitive alternative to retrieve AOD with acceptable accuracy. For instance, in recent research (García-Cabrera et al., 2020; Gröbner and Kouremeti, 2019; Qiao et al., 2023), an EKO MS-711 collimated spectroradiometer was used to retrieve AOD at multiple wavelengths. Chapter 6 is dedicated to implement a method of retrieval of AOD at different wavelengths from EKO MS-711 ground measurements of direct normal spectral irradiance. This represents a first step towards acquiring local experience on retrievals of atmospheric parameters.

1.2. Objectives

The objectives of this work are:

- **Over-irradiance:** to determine how often OIE occur in Uruguay, what is their typical duration, intensity, magnitude and distribution in this region throughout the seasons and daytime.
- **Physical clear-sky models SMARTS and REST2:** to implement and evaluate the accuracy of these physical clear-sky models (one spectral, the other broad-band) in Uruguay, and to determine what is their performance against ground measurements of spectral and broadband irradiance, in their products of Global, Diffuse and Beam. It is also relevant to determine the most adequate sources for atmospheric information.
- **Retrievals of AOD:** to apply an inversion algorithm on collimated beam spectroradiometer ground measurements taken at Montevideo's AERONET site and evaluate the accuracy of this retrieval against the independent simultaneous ground measurements from AERONET.

Finally, in a more ambitious pursuit, the overall aim of this work is to be of use to anyone interested in approaching simplified physical models of irradiance (such as SMARTS or REST-2), or retrievals of atmospheric parameters (such as aerosol optical depth) from ground measurements, offering a balanced compromise between theoretical and technical aspects needed to find the answers to the typical problems faced.

1.3. Organization of this thesis

Chapter 2, supplemented by Appendix B, provides essential concepts to contextualize the results that will be presented in later chapters, related to solar radiation in the atmosphere. Additionally, the data required for the chosen methodologies is described, such as satellite sources, reanalysis data bases and ground measurements. Chapter 3 is dedicated to the first statistical characterization of over-irradiance events (OIE) in Uruguay. This chapter is an updated version of work presented at the 2021 ISES Solar World Congress (Russo et al., 2021), showing additional results. Chapter 4 is dedicated to the spectral irradiance model SMARTS, under clear-sky conditions, (Gueymard, 1995, 2019). It gives an overlook of its algorithm, explores its sensitivity to variations in relevant input atmospheric parameters and reviews its previous performance results. Then it describes and implements an original methodology (based on the sun and shade method) used to obtain global and diffuse measurements from the same instrument. SMARTS performance is analysed against ground measurements, of 1 minute sampling interval, with different sources of atmospheric inputs. Chapter 5 is focused on the related broadband irradiance model REST2 (Gueymard, 2008b), under clear-sky conditions. This chapter is an improved and updated version of work presented at the CBENS 2022 (Russo et al., 2022) with some improvements applied. It provides a brief overview of its two-band algorithm, and presents a performance analysis of its estimates for Global, Diffuse and Beam irradiance, at 1 minute sampling interval for a 4 years data set of ground measurements. Different sources of atmospheric information are considered. Chapter 6, adapted from (Russo et al., 2023), is dedicated to the estimation of AOD at six wavelengths (concordant with AERONET's measurements), using an inversion or retrieval algorithm applied to ground measurements of beam spectral irradiance taken with a collimated spectroradiometer (EKO MS-711). The algorithm is based on the combination of the Lambert-Beer-Bouguer Law with the Langley plot method. The retrieval results are presented and compared against AOD from AERONET. Finally, Chapter 7 presents a general discussion of the results obtained and the goals achieved, with an overview of future work.

Chapter 2

Solar Radiation in the Atmosphere

In this chapter, the notation and required basic concepts are briefly reviewed. The sources of surface and atmospheric information used in this thesis are described and the basic performance metrics are introduced. Specific details are discussed in Appendices A and B, both of which complement this summary.

2.1. Fundamental concepts of solar radiation

Irradiance

Spectral radiance L_λ ($\text{W m}^{-2} \text{sr}^{-1} \text{nm}^{-1}$), (ISO 9488:2022, 2022), is the radiant power dP (W) per unit of projected area $dA \cos \theta$ (m^2), per unit of solid angle $d\Omega$ (in steradians, sr), per unit of wavelength $d\lambda$ (nm) received on a differential surface element dA , as shown in Eq. (2.1). In this context, the angle of incidence θ (rad) is defined as the angle between the direction of incidence and the normal to the surface element, as shown in Fig. (2.1),

$$L_\lambda = \frac{dP}{\cos \theta \, dA \, d\Omega \, d\lambda}. \quad (2.1)$$

Consequently, the solar spectral irradiance incident on a horizontal surface, $G_{h,\lambda}$ ($\text{W/m}^2\mu\text{m}$) (the solar spectral wavelength range is approximately 280-4000 nm), is obtained by integrating the spectral radiance L_λ in all directions within a hemisphere above the surface. Integration is performed accounting for the angular distribution of incoming radiation and the solar zenith angle, θ_z ¹ (rad); where θ_z is the angle between the Sun-Earth direction and the local normal (Duffie and Beckman, 2006). It returns the power incident on a surface per unit area, per wavelength

$$G_{h,\lambda} (\text{W/m}^2\mu\text{m}) = \int_{\Omega} L_\lambda \cos \theta_z \, d\Omega. \quad (2.2)$$

¹For a horizontal receiving surface, the incidence angle θ coincides with the solar zenith angle θ_z . For arbitrarily tilted surfaces, these angles are generally different.

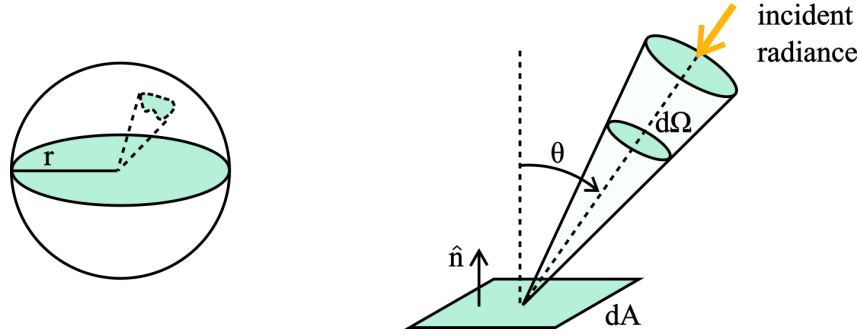


Figure 2.1: Irradiance concept and components. Adapted from Wald (2020).

If $G_{h,\lambda}$ ($\text{W}/\text{m}^2\mu\text{m}$) is integrated over the solar spectral range (280-4000 nm), then the broadband irradiance, G_h (W/m^2) is obtained

$$G_h (\text{W}/\text{m}^2) = \int_{\lambda} G_{h,\lambda} d\lambda. \quad (2.3)$$

Solar irradiance at the top of the atmosphere (TOA)

The solar irradiance incident at TOA is not constant, partly because the Sun undergoes periodic cycles of higher and lower activity. To account for this variability, the long-term average of the solar irradiance at a distance of 1 A.U.² from the Sun is considered. This quantity is known as the solar constant, G_s , and its currently accepted value is $1361 \text{ W}/\text{m}^2$ (Prša et al., 2016). This value has been established based on an average of several years of satellite irradiance measurements at TOA normalized to the mean Sun-Earth distance of 1 A.U., since its variability is smaller than approximately 0.3 % (Kopp and Lean, 2011).

The solar flux incident at TOA depends quadratically on the Sun-Earth distance (r). This is accounted for with the orbital correction factor $F_n = (r_0/r)^2$ (Duffie and Beckman, 2006; Iqbal, 1983), where $r_0 = 1 \text{ A.U.}$ is the average Sun-Earth distance,

$$F_n \equiv \left(\frac{r_0}{r}\right)^2 \simeq 1 + 0.033 \cos\left(\frac{2\pi n}{365}\right), \quad (2.4)$$

where n is the ordinal day of the year, between 1 and 365 for normal years. Other formulas to estimate F_n with greater precision have also been proposed, among them, (Spencer, 1971) shown in Eq. (B.1), which is a parametric formula derived from Fourier series. F_n is independent of solar activity and accounts for a variation of about 3.3 % in the TOA irradiance, so it is not negligible as opposed to solar activity variations.

²One astronomical unit (A.U.) corresponds to the mean Sun-Earth distance.

The horizontal irradiance received at TOA is then

$$G_{0h} = G_s F_n \cos \theta_z = G_0 \cos \theta_z, \quad (2.5)$$

where G_0 (W/m^2) is the solar irradiance at TOA in normal incidence. This equation also holds for TOA spectral irradiance $G_{0,\lambda}$ ($\text{W/m}^2\mu\text{m}$), replacing the solar constant with a standard solar spectrum at 1 A.U., $G_{s,\lambda}$ ($\text{W/m}^2\mu\text{m}$). Several standard solar spectrums at TOA are in use (Gueymard, 2004; Wehrli, 1985).

Direct and diffuse radiation

From the point of view of an observer at ground level, Global Horizontal Irradiance (G_h in broadband terms, or $G_{h,\lambda}$ in spectral terms) is the sum of two irradiance components. One of these components is the beam normal irradiance (G_b in broadband terms or $G_{b,\lambda}$ in spectral terms) projected onto a horizontal plane, and the other is the diffuse horizontal irradiance (G_{dh} in broadband terms or $G_{dh,\lambda}$ in spectral terms). This relationship is expressed by the closure equation (Eq. 2.6), which is valid in both broadband and spectral terms,

$$\begin{aligned} G_h &= G_{dh} + G_b \cos \theta_z, \\ G_{h,\lambda} &= G_{dh,\lambda} + G_{b,\lambda} \cos \theta_z. \end{aligned} \quad (2.6)$$

Since the spectral quantities $G_{h,\lambda}$, $G_{dh,\lambda}$ and $G_{b,\lambda}$ represent irradiances expressed as functions of wavelength, their broadband versions are obtained by integrating over the solar spectral range. Therefore, the broadband closure follows directly from the integration of the spectral closure relation, according to Eq. (2.3). This is possible because the projection factor $\cos \theta_z$ is independent of wavelength, while the spectral modifications introduced by atmospheric extinction are already contained in $G_{b,\lambda}$.

G_b ($G_{b,\lambda}$) is the irradiance (spectral irradiance) that would be measured if a narrow cone with its axis aligned with the Earth-Sun direction, including the Sun's disc and a narrow surrounding area (circumsolar region), was placed at ground level. The instruments specifically designed to measure G_b are called pyrheliometers. The instruments designed to measure $G_{b,\lambda}$ are spectroradiometers with a collimator tube. Sunphotometers also measure $G_{b,\lambda}$ in certain spectral windows. As shown in Fig. 2.2, the apparent angular diameter of the solar disc outside the atmosphere varies between approximately 0.526° and 0.545° due to orbital eccentricity (Andreas, 2021). However, under atmospheric conditions, the size of the solar disc varies between 3° and 7° , depending on the atmospheric turbidity. For this reason, pyrheliometers use a Field of View (FOV) of 5° by convention, as recommended by (ISO 9060:2018(E), 2018; World Meteorological Organization (WMO), 2023).

G_{dh} ($G_{dh,\lambda}$) is the irradiance (spectral irradiance) that comes from all the other hemispherical directions not included in the G_b cone. Since the atmosphere is composed by gas molecules, aerosol particles, water vapour, droplets and crystals, when a photon reaches the atmosphere,

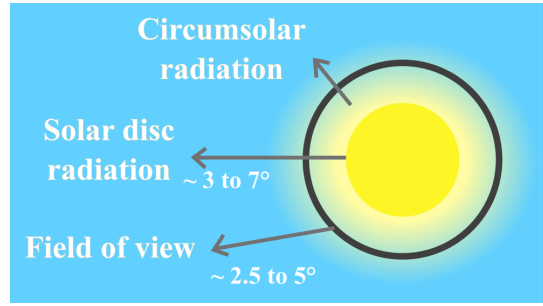


Figure 2.2: Circumsolar radiation. Note the field of view depends on the measurement instrument. (Figure not to scale). Figure by Paola Russo.

there is a certain probability that it encounters particles and/or gases on its way to the ground surface, which produce events of reflection and scattering, contributing to diffuse irradiance.

Two useful dimensionless parameters are: the diffuse fraction f_d (Eq. 2.7) and the clearness index k_t (Eq. 2.8). Both parameters are commonly used to characterise atmospheric conditions in the context of solar radiation models. f_d provides a relative estimate of the fraction of incident global irradiance that has been scattered, while k_t is a normalized form of global irradiance,

$$f_d = G_{dh}/G_h, \quad (2.7)$$

$$k_t = G_h/G_{0h}. \quad (2.8)$$

In practice, k_t is strongly related to cloudiness, under clear-sky conditions it tends to take values close to 0.85 to account for the attenuation of a clear atmosphere, while during overcast situations it may decrease to almost zero. Similarly, f_d increases with the presence of clouds, with values close to 0.10 for clear skies and approaching 1 in fully overcast conditions.

Spectral characteristics of solar radiation

Fig. 2.3 represents solar spectral irradiance before and after passing through the atmosphere. If the Sun is assumed to be a black body, its surface temperature can be estimated as approximately 5777 K (Mamajek et al., 2015). It emits radiation in a wavelength range of 100 to 4000 nm, usually divided into spectral regions for their study. Since region labels may correspond to slightly different intervals in the literature, Table 2.1 defines the ranges adopted in this work, to avoid any ambiguity. The solar irradiance for each band is obtained integrating the spectral irradiance in the spectral region of interest,

$$G_{h, [\lambda_1, \lambda_2]} (\text{W/m}^2) = \int_{\lambda_1}^{\lambda_2} G_\lambda d\lambda. \quad (2.9)$$

Some particular characteristics of each band are outlined below.

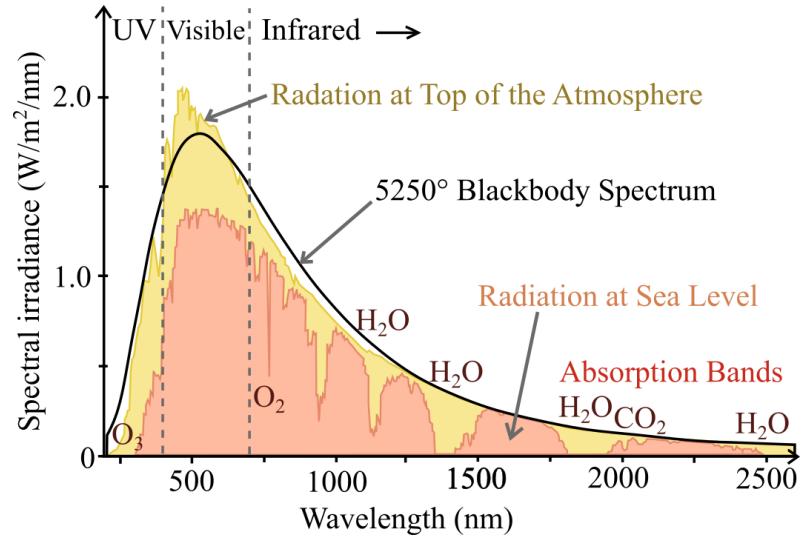


Figure 2.3: Solar spectrum at TOA (yellow), blackbody approximation (black line) and typical beam solar spectrum at sea level under clear-sky (red). Adapted from: (Rohde, 2008).

Description	Band	Wavelength range (nm)	f_b (%)
Ultraviolet	UV-C	100-280	~ 0
Ultraviolet	UV-B	280-315	1.3
Ultraviolet	UV-A	315-400	6.2
Photosynthetically Active Radiation	PAR	400-700	39.2
Near Infrared	NIR	700-1000	22.6
Infrared	IR	1000-2500	27.2
Thermal radiation		2500- ∞	2.5

Table 2.1: Wavelength bands as adopted in this work. The last column f_b , shows each band's fraction of total solar irradiance, according to Wehrli (1985).

- UV-C: between 100 and 280 nm, this radiation does not reach the Earth's surface because it is fully absorbed by molecular oxygen and ozone in the higher layers of the atmosphere.
- UV-B: between 280 and 315 nm, is mainly absorbed by ozone and only approximately 5 % of it reaches the ground surface (Aggarwal et al., 2013). It is related to damages to human skin tissues and eyes, therefore it is of wide interest in human health (Lucas et al., 2006).
- UV-A: between 315-400 nm, is weakly absorbed by stratospheric ozone, resulting in nearly 95 % of it reaching the ground surface (Aggarwal et al., 2013). It contributes to materials degradation (Shamachurn and Betts, 2016) and human health problems such as skin ageing, cataracts, melanoma, among others (Lucas et al., 2006). Nevertheless, a certain

amount of this radiation is necessary for the human body in order to synthesise vitamin D (Holick, 2004; Webb et al., 1988).

- Visible (VIS) or Photosynthetically Active Radiation (PAR): between 400 and 700 nm, corresponds to the portion of the spectrum that is detectable by the human eye and may be used by plants for photosynthesis. Notice that almost 40 % of the incident solar irradiance is accounted as beam irradiance in this band. It is of particular importance in crop productivity and agrivoltaic applications (AL-agele et al., 2021; Habyarimana et al., 2019).
- Near Infrared (NIR): is between 700 and 1000 nm, it is usually of interest in climate and Earth's energy budget applications (Feldman et al., 2014). In the atmosphere, NIR irradiance is weakly scattered and is primarily absorbed by H₂O in specific spectral regions (see Fig. 2.3).
- Infrared (IR) and thermal radiation: is between 1000 and 4000 nm. It is a region where the intensity drops as the wavelength grows. Absorption in this region is mainly caused by water vapour and CO₂.

As mentioned, the exact ranges may vary slightly, depending on the Norm or source that defines them.

2.2. Solar radiation in the atmosphere

Scattering and absorption

As radiation passes through the atmosphere, it can interact with various atmospheric constituents, including major gases (such as molecular oxygen, O₂, and molecular nitrogen, N₂), aerosols (suspended particles of diverse shapes, sizes, and origins, such as mineral dust, sea salts, and biomass burning residues), water vapour and ice crystals, ozone (O₃), and trace gases (such as nitrogen dioxide, NO₂, carbon dioxide, CO₂). These particles and molecules attenuate the incoming solar beam primarily due to two radiative processes: scattering and absorption, as shown in Fig. 2.4.

Scattering

Scattering refers to the interaction between a photon and an atmospheric particle, in which the photon's direction of propagation typically changes. In atmospheric contexts, scattering is typically elastic, meaning that the photon's wavelength and energy remain unchanged during the interaction. Depending on the relationship between the wavelength (λ) and the size of the particle, scattering can be described by different theoretical frameworks: Rayleigh Scattering

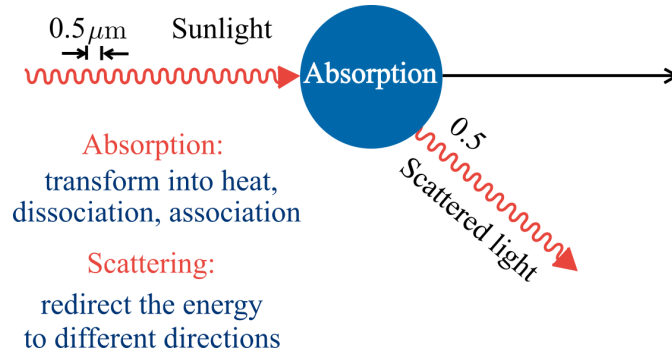


Figure 2.4: Simplified scheme of the absorption and scattering process. Adapted from (Mikuška, 2013).

(Strutt, 1871), Mie Theory (Mie, 1906), and Geometric Regime (van de Hulst, 1957). This relationship is expressed through the size parameter (x) (Eq. 2.10), which depends on the particle's effective diameter (D) and the incident photon wavelength (λ),

$$x = \frac{\pi D}{\lambda}. \quad (2.10)$$

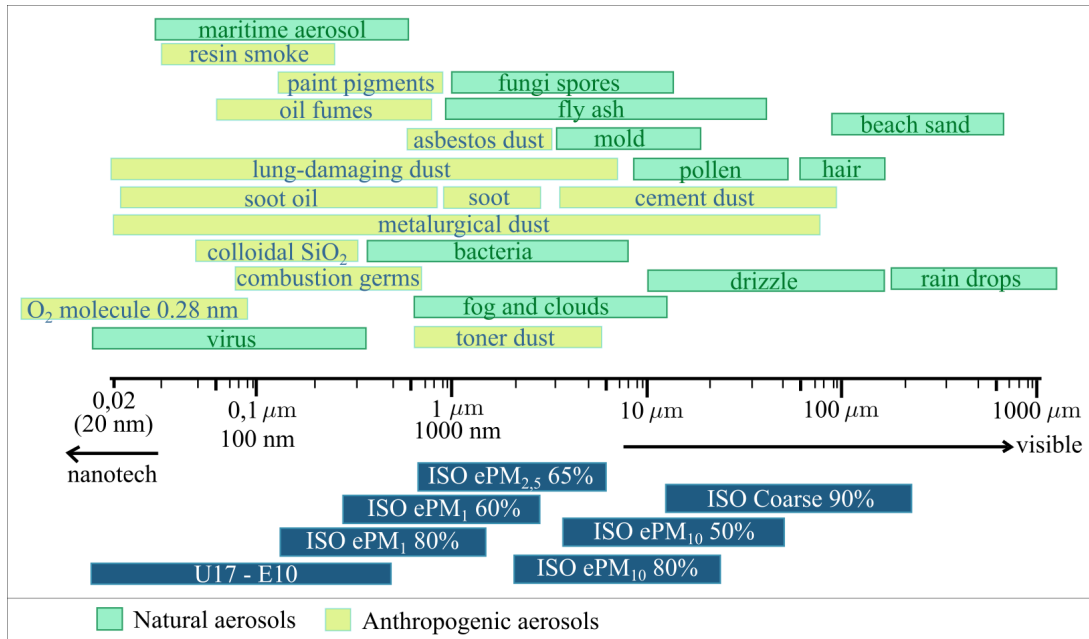


Figure 2.5: Particle size of different atmospheric components. Adapted from: (ISO 16890-2:2022, 2022). ePM: efficiency of particulate matter.

In scattering theory, particles are typically approximated as spheres with an effective diameter D . Fig. 2.5 illustrates various aerosol components and their characteristic sizes. Based on particle size, they are commonly classified according to (ISO 16890-2:2022, 2022) as: suspended particles (size smaller than $0.4\text{ }\mu\text{m}$ and typically labelled in the Particulate Matter 1 category, PM_1), fine particles (size up to $10\text{ }\mu\text{m}$ and typically labelled in the PM_{10} category), and coarse particles (sizes larger than $10\text{ }\mu\text{m}$). Fig. 2.6 shows the characteristic scattering patterns produced in each regime as a function of the size parameter x .

i) Rayleigh Scattering: is applicable when particles are much smaller than the incident wavelength ($x \ll 1$). Rayleigh scattering theory relies on idealised assumptions: the particles are treated as infinitesimal dipoles, the medium is non-absorbing and isotropic, and the scattering is elastic. For example, this model is usually applied to air molecules (mainly composed of O_2 and N_2). The dispersion pattern generated in this regime is shown in Fig. 2.6 (a), where the photons that hit the particle can be redirected with equal preference to the back and forward directions of the beam and with a smaller probability of scattering in a plane perpendicular to the incident direction. In this case, the probability of scattering is proportional to λ^{-4} , which means that smaller wavelengths will present larger scattering. As a result, the blue colour, which is one of the shortest wavelengths visible to the human eye ($450\text{--}495\text{ nm}$), is more efficiently scattered in all directions than the other colours (compared to red, for instance, located around $620\text{--}750\text{ nm}$). This causes the sky to appear blue during clear-sky days, and it is also the reason why clear atmospheres are called Rayleigh atmospheres. Furthermore, Rayleigh theory also explains why sunsets and sunrises look in the tones of red, orange and yellow. When the sun is close to the horizon line, photons travel through a larger path length, encountering a greater amount of molecules. This causes the blues to vanish from the incident beam and the reds to be enhanced, as they correspond to longer wavelengths less affected by scattering.

ii) Mie Theory: is applicable when the particle size is greater than λ (implying $x \geq 1$). This is, for example, the case of aerosols, fog, or volcanic ash, as shown in the centre of Fig. 2.5. These particles are usually located in the troposphere (lower layer of the atmosphere, from the ground to about 2 km altitude). Mie Theory supposes that particles can be modelled as a homogeneous sphere, and statistically, the estimates scattering has a lobular pattern (similar to Rayleigh's scattering but with more pronounced lobules). As shown in Fig. 2.6 (b), there is a higher probability for the photons to scatter forward along the incident direction, and low probability of the photons to disperse in the plane perpendicular to the incidence direction. Particles with sizes larger but comparable to the wavelength of the photon produce a scattering that depends less on the wavelength and more on the particle size, resulting in a scattering that is only weakly colour selective and has a strong forward direction. This explains the milky or greyish appearance of foggy skies.

iii) Geometric Optics Regime: is applicable when the particle is large compared to λ ($x \gg 1$). For example, this is the case of water droplets or ice crystals, as shown on the right side of Fig. 2.5. The phenomenon is governed by reflection and refraction. A representation of

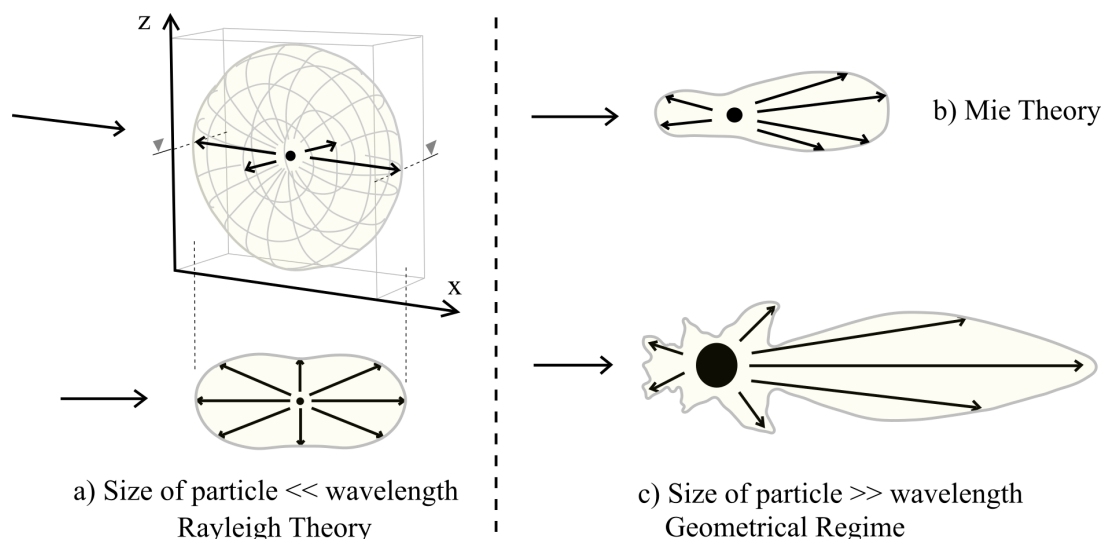


Figure 2.6: Scattering patterns. Adapted from: (Bunge et al., 2006; Wald, 2020)

the statistical estimation of the dispersion pattern is shown in Fig. 2.6 (c), where the photon has a high probability of being dispersed forward. Therefore, in the geometric optics regime, where particles such as water droplets or ice crystals are much larger than the wavelength of the photon, scattering is governed by reflection, refraction and diffraction, leading to optical phenomena like halos and rainbows, due to the structured interaction of photons with spherical particles.

Absorption

When a photon is absorbed by a molecule, its energy is converted into vibrational or kinetic energy (heat) which can drive photochemical reactions such as molecular dissociation or recombination. As mentioned above, it is caused mainly by gas molecules and aerosols. Absorption by a given compound is a spectrally selective process. This property is used in spectrophotometry to identify the presence or absence of a compound in a continuous and homogeneous medium that is being illuminated. In the particular case of the atmosphere, the goal of some applications is to identify the presence of a specific atmospheric component and estimate its optical depth (defined in Eq. 2.15). For instance, Figure 2.3, shows the absorption effects from water vapour, mainly in the NIR and IR bands. Figure 2.7 shows the absorptivity, defined as the fraction of incident radiation that is absorbed by each radiatively active gas in the atmosphere. Observe particularly how water vapour (H_2O) absorbs around the wavelength of 935 nm (among other wavelengths), whereas the other atmospheric components show negligible absorption in this band. That distinctive absorption characteristic is what allows to use retrieval techniques applied around that wavelength to estimate precipitable water vapour.

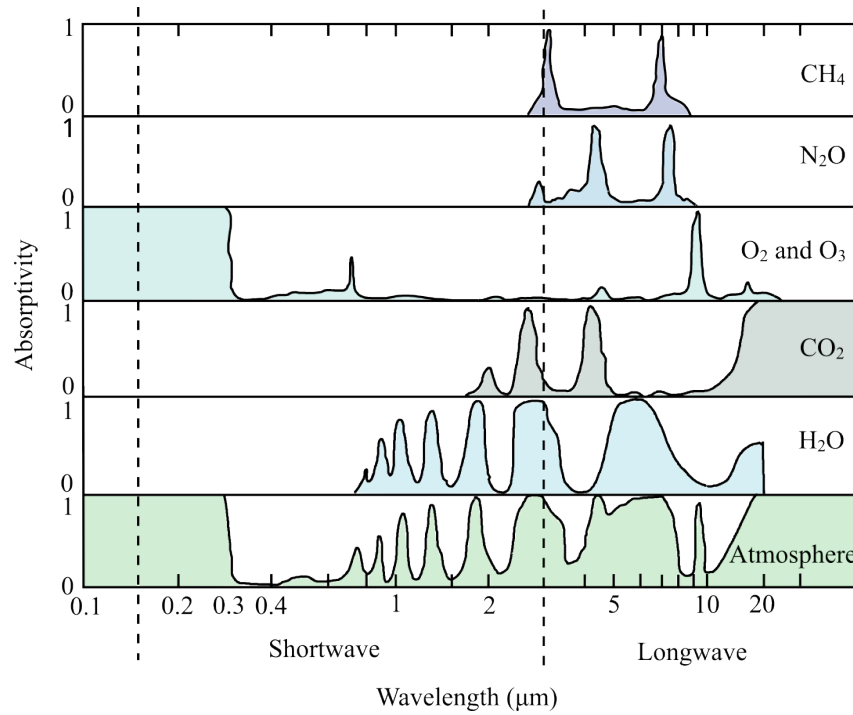


Figure 2.7: The absorption of short wave and long wave radiation due to radiatively active gases in the atmosphere happens in different wavelengths. Adapted from (Peixoto and Oort, 1992).

Air mass

As discussed in previous sections, the attenuation of a radiation beam depends on various factors, such as the number, size, shape, and surface properties of the molecules and particles encountered along its path. Consequently, the overall effect is determined not only by these particle characteristics but also by the air's volumetric density and the length of the optical path, which are related to the total number of interactions.

A useful parameter to describe this is the relative air mass. Since the volumetric density ρ (kg/m^3) of the atmosphere varies with altitude, ρ can be expressed either as a continuous function of vertical height z , $\rho(z)$, or as a function of the slant path s , $\rho(s)$. Additionally, the number density, n (m^{-3}), is the number of particles N , contained in a unit volume V (m^3). n can be converted into ρ by multiplying by the mass of the particle m_p (kg). Thus analogously to ρ , the number density can be expressed as $n(z)$ or as $n(s)$. The absolute air mass along a slant path σ , is defined as: $\sigma = \int_1^2 \rho(s) ds$, being 1= TOA and 2= ground level (GND). Similarly, the absolute air mass at the zenith, σ_z , is obtained by integrating over a vertical path: $\sigma_z = \int_1^2 \rho(z) dz$. The relative optical air mass m , is then defined as the ratio between the absolute air mass along the

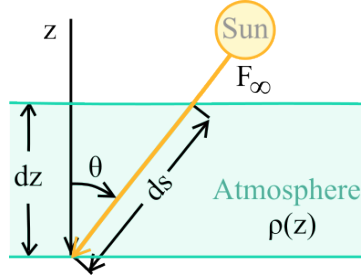


Figure 2.8: Air mass scheme. Figure by Paola Russo.

slant path and the absolute air mass at the zenith:

$$m = \frac{\sigma}{\sigma_z} = \frac{\int_1^2 \rho(s) ds}{\int_1^2 \rho(z) dz} = \frac{\int_1^2 n(s) ds}{\int_1^2 n(z) dz}. \quad (2.11)$$

Since the atmospheric density profiles are in principle different from each atmospheric component, the relative air mass is component-specific (see Fig. 2.9). A particular case is the single layer model of a plane-parallel atmosphere, without refraction effects, which assumes that the density only varies with height. In this case, $ds = dz / \cos \theta_z$, and the relative air mass simplifies to

$$m = 1 / \cos \theta_z \text{ (unitless)}. \quad (2.12)$$

This expression has a geometric interpretation, as shown in Fig. 2.8: it represents the optical path length of sunlight through the plane atmosphere relative to the path length when the Sun is at the zenith. At a zenith angle of $\theta_z = 0^\circ$, the relative air mass is $m = 1$. As the zenith angle increases, m also increases, for example, at $\theta_z = 60^\circ$, $m \approx 2$, and near $\theta_z \rightarrow 90^\circ$ Eq. (2.12) fails and m diverges.

When the zenith angle is not too large, the plane layered atmosphere provides an acceptable approximation, and the relative air mass can be calculated with Eq. (2.12), (Iqbal, 1983). However, for zenith angles larger than 70° , this equation becomes inaccurate due to diffraction effects and the Earth's sphericity. To address this limitation, parametric expressions for m that include empirical corrections to the solar zenith angle have been developed, as illustrated in Fig. 2.9. One of these expressions is proposed by (Young, 1994),

$$m = \frac{1.002432 \cos^2 \theta_z + 0.148386 \cos^2 \theta_z + 0.0096467}{\cos^3 \theta_z + 0.149864 \cos^2 \theta_z + 0.0102963 \cos \theta_z + 0.000303978}. \quad (2.13)$$

Specific relative air masses have been parameterized for extinctions associated with each atmospheric component (aerosols, gases, water vapour), since they have different density profiles in the atmosphere. In these cases, Eqs. (B.2) to (B.5) from Appendix B.2, provide greater precision for zenith angles nearer the horizon, and for each individual atmospheric component.

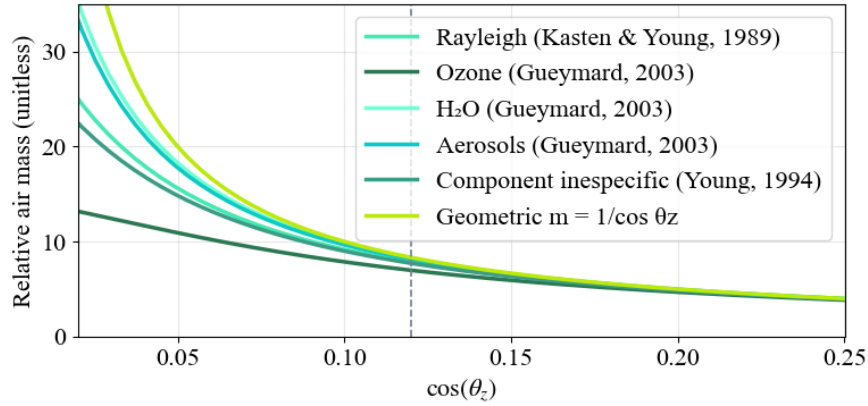


Figure 2.9: Relative air mass parametrizations for several atmospheric components. Figure by Paola Russo.

Spectral optical depth

The spectral extinction cross section σ_λ (m^2) represents the effective area of interaction between a single particle and the incident radiation beam at wavelength λ . It quantifies the ability of the particle to attenuate radiation through both scattering and absorption processes. It depends on the spectral scattering cross section $\sigma_{s\lambda}$ (m^2), and the spectral absorption cross section $\sigma_{a\lambda}$ (m^2):

$$\sigma_\lambda = \sigma_{s\lambda} + \sigma_{a\lambda}. \quad (2.14)$$

Consider an incident radiance beam coming from the sun, as shown in Fig. 2.10. The path s , that goes in the direction of propagation (grows towards the ground), has a differential length ds and forms an angle θ_z with the local vertical.

Using the previous concepts, the differential optical depth can be defined as $d\tau_\lambda = \sigma_\lambda n(z) dz$. The total spectral optical depth, τ_λ (unitless), is then obtained by integrating the differential optical depth from the top of the atmosphere (TOA) to the ground (GND), as shown in Eq. 2.15. Therefore, τ_λ is zero at TOA and reaches a maximum value of τ_λ at ground level.

$$\tau_\lambda = \sigma_\lambda \int_{TOA}^{GND} n(z) dz \quad (2.15)$$

Thus, the spectral optical depth is the product of the column density and the interaction probability of the component at the relevant wavelength.

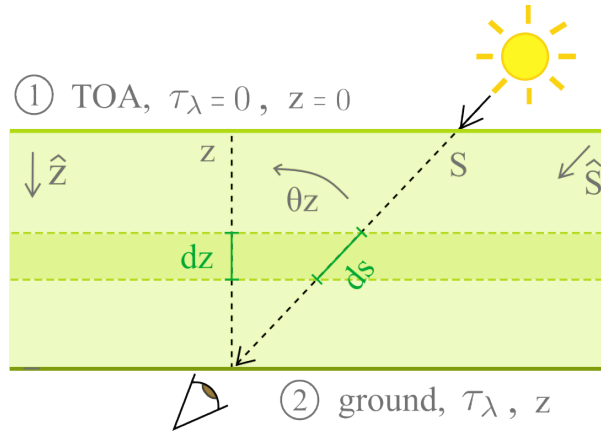


Figure 2.10: Plane atmosphere representation for the optical depth, RTE and Lambert Law. Figure by Paola Russo.

Radiative transfer equation (RTE)

The radiative transfer equation (RTE) describes the differential change in the spectral radiance L_λ as it travels along a path ds . This change is caused by an added quantity of radiance in the beam ($dL_{a\lambda}$), that comes from emission and scattering elsewhere, also known as the source function, and a removed quantity from the beam ($-dL_{r\lambda}$), that is caused by extinction, which includes absorption and scattering out of the beam,

$$dL_\lambda = dL_{a\lambda}(\text{added}) - dL_{r\lambda}(\text{removed}). \quad (2.16)$$

The amount of radiation removed from the beam is proportional to the current radiance (L_λ), σ_λ , $n(s)$ and ds , obtaining: $dL_{r\lambda} = \sigma_\lambda n(s) L_\lambda ds$. The amount of radiation added to the beam is described by the spectral volume coefficient (j_λ), which includes thermal emission and scattered radiation into the path, and is expressed as: $dL_{a\lambda} = j_\lambda ds$. Combining the two terms leads to the differential form of the general Equation of Radiative Transfer (ERT, Eq. 2.17):

$$\frac{dL_\lambda}{ds} = j_\lambda - \sigma_\lambda n(s) L_\lambda. \quad (2.17)$$

In its general form, the ERT accounts for both attenuation and incoming scattering/emission processes through the source term j_λ . However, in the applications considered in this work, the equation is applied to direct solar radiation within the solar spectral range. Under these conditions, the thermal emission by the atmosphere is imposed to be negligible, and the radiation scattered into the beam direction is not explicitly modeled. Therefore, the source term j_λ is neglected in the following developments.

Lambert's Law

The Lambert's Law (historically attributed Lambert, Beer and Bouguer) describes the exponential attenuation of a solar irradiance beam as it transverses an homogeneous atmosphere with a single component gas and reaches the ground. This formulation takes into account the air mass and contributions from different atmospheric components. Consider an incident beam of irradiance coming from the Sun that transverses the atmosphere, as shown in Fig. 2.10. For the following deduction to be valid, the atmosphere does not need to be plane parallel, even though in Fig. 2.10 the TOA and ground limits are represented as straight lines. As described in Section 2.2, the slant path is s , the vertical path is z , and both increase from TOA towards the ground. The beam of irradiance is attenuated by the particles present in the atmosphere, since they have a certain probability of intercepting the photons, causing scattering and absorption. The attenuation is proportional to the probability of interaction, the density of gas molecules and the intensity of the beam:

$$dG_{b,\lambda} = -\sigma_\lambda G_{b,\lambda} n(s) ds. \quad (2.18)$$

Notice that this represents a special case of the RTE (Eq. 2.17) in which the source function is neglected. Rearranging Eq. 2.18 and integrating it from TOA to GND yields

$$\int_{TOA}^{GND} \frac{dG_{b,\lambda}}{G_{b,\lambda}} = -\sigma_\lambda m \int_{TOA}^{GND} n(z) dz. \quad (2.19)$$

Integration of both sides of Eq. (2.19) yields the exponential attenuation (Lambert's Law):

$$G_{b,\lambda} = G_{0,\lambda} e^{-\tau_\lambda m}. \quad (2.20)$$

A useful parameter that appears in this equation is the spectral transmittance $T_\lambda = G_{b,\lambda}/G_{0,\lambda}$ (unitless). If the Lambert Law applies, then T_λ is:

$$T_\lambda = e^{-\tau_\lambda m}. \quad (2.21)$$

In order to use Eq. (2.20), irradiance models must specify which atmospheric species are considered and how their air mass and optical depth are represented. In this context, simplified radiative transfer models, such as those employed in this thesis in Chapters 4, 5 and 6 (SMARTS, REST-2, retrievals of AOD), adopt the following assumptions. First, the atmosphere behaves as composed of consecutive layers where the following attenuation processes happen: Rayleigh scattering (r), ozone absorption (o), nitrogen dioxide absorption (n), uniformly mixed gases attenuation (g), water vapour absorption (w), aerosol attenuation (a). Second, those processes are independent from each other (or in other words, the interaction between them is neglected). Taking this into account, the total transmittance (Eq. 2.21) becomes a product of transmittances, which can be expressed as

$$T_\lambda = T_{r\lambda} T_{o\lambda} T_{n\lambda} T_{g\lambda} T_{w\lambda} T_{a\lambda} = e^{-\sum_i \tau_{\lambda i} m_i}. \quad (2.22)$$

Ångström's Law

To quantify the aerosol contribution to the shortwave attenuation described by Lambert's Law, the aerosol optical depth $\tau_{a\lambda}$ can be estimated using Ångström's Law, which provides a simple empirical relationship between the aerosol optical depth and wavelength. Using a reference wavelength $\lambda_1 = 1 \mu\text{m}$, the aerosol optical depth at any wavelength λ can be expressed as

$$\tau_{a\lambda} = \beta \lambda^{-\alpha}, \quad (2.23)$$

where α (unitless) is the Ångström exponent, related to the particle size distribution (higher values indicate dominance of fine particle aerosols, lower values indicate large particle aerosols), and β (unitless) is the Ångström turbidity coefficient, which is the aerosol optical depth at $\lambda = 1 \mu\text{m}$ and quantifies the aerosol load in the atmosphere. Typical values for a clean atmosphere are $\alpha = 1.30$ and $\beta = 0.20$ (Iqbal, 1983).

This equation allows to calculate $\tau_{a\lambda}$ at any given wavelength, if α and β have previously been estimated at two wavelengths λ_1 and λ_2 . For the inverse problem, if $\tau_{a\lambda}$ is known at two or more wavelengths, α can be estimated from Eq. (2.24) as

$$\alpha = -\frac{\log(\tau_{a\lambda_1}/\tau_{a\lambda_2})}{\log(\lambda_1/\lambda_2)}. \quad (2.24)$$

Retrieval or Inversion Algorithms

Atmospheric parameters such as AOD, integrated water vapour profile or total columnar ozone, can be estimated from solar spectral irradiance measurements using retrieval or inversion algorithms (Rodgers, 2000). As mentioned before, the general idea consists in retrieving the desired parameter, for example $\tau_{a\lambda}$, from Eq. 2.20.

These techniques normally require having precise monochromatic irradiance measurements from sunphotometers or spectroradiometers. They can be implemented for both ground measurements and satellite measurements, and the working principle remains the same, however, specific complexities are characteristic of each technique. For example, the products of aerosol optical depth available from Plankton, Aerosol, Cloud, Ocean Ecosystem (PACE mission, NASA ³) are calculated using inversion techniques on measurements from a hyperspectral imaging radiometer on board of a satellite. Furthermore, the aerosol optical depth products available from AERONET (see Section 2.4) are calculated using retrieval algorithms applied to spectral irradiance measurements taken with sunphotometers at ground level.

Retrieval algorithms are implemented at specific wavelengths because they rely on the principle that different atmospheric components have spectrally selective interactions with incident solar photons. Wavelengths are carefully chosen to maximize sensitivity to the target while minimizing

³<https://pace.gsfc.nasa.gov/>

interference from other species or surface reflectance effects, ensuring more accurate and stable retrievals. Retrievals can be performed over different components, for example, ozone, aerosols, water vapour. This thesis will be focused on aerosol retrievals specifically. Chapter 6 shows the retrieval of AOD at various wavelengths from ground measurements, using these ideas.

2.3. Over-irradiance or cloud enhancement

Over-irradiance (OI) events are a well known short term phenomena characterized by a rapid increase of global irradiance values (G_h) above the expected clear-sky value. These events can last several minutes and result in global irradiances which are larger than those at the top of the atmosphere (TOA). G_h values in excess of 1400 W/m^2 , 1650 W/m^2 , 1634 W/m^2 or even 1691 W/m^2 have been registered on the 1-minute timescale at different sites (Castillejo-Cuberos and Escobar, 2020; de Andrade and Tiba, 2016; Gueymard, 2017; Inman et al., 2016). OI events are also known as cloud enhancement events, since they are due to an enhancement of the diffuse irradiance component of global irradiance by the effects of the cloud distribution under partially cloudy conditions. However, fluctuations in beam irradiance may exceptionally be present (Gueymard, 2017).

OI events have several practical implications, and they occur more commonly than one may think. For example, in photovoltaic plants, OI events raise the generator current, stressing protection systems and accelerating inverter degradation. This may lead to shorter inverter lifespans and higher operation costs (Toreti et al., 2021). OI peaks in the power generated are difficult to account by forecasting models (Gueymard, 2017; Järvelä et al., 2020). OI can also affect human health, because when over irradiance events occur, the irradiance intensity at the UV region of the spectrum is also enhanced (Feister et al., 2015), increasing the risk of its impacts on human skin and eyes. For the same reason, OI combined with other environmental factors such as temperature and humidity can lead to photo-oxidation of the nowadays extensively used polymers, which contributes to environmental pollution, impacting ecosystems (Zhang et al., 2024).

Different cloud configurations can physically cause over-irradiance (Mol and Van Heerwaarden, 2025). Opaque clouds such as altocumulus can generate strong irradiance spikes through forward scattering. Flat, optically thick clouds like stratus enhance irradiance directly beneath them by diffuse downward scattering, while vertically developed convective clouds may induce strong lateral enhancements that can extend tens of kilometres from the cloud edge. In addition, multiple scattering between the surface and optically thick clouds leads to albedo-driven irradiance increases, particularly over bright surfaces. Together, these mechanisms explain why broken, stratified, and vertically developed cloud fields are frequently associated with over-irradiance events. As an example, Figure 2.11 shows how the phenomenon looks like for the case of cirrus clouds and cumulus, stratocumulus clouds.

Previous studies have consistently shown that solar over-irradiance (OI) events, loosely defined



(a) Cirrus clouds.



(b) Cumulus, stratocumulus clouds.

Figure 2.11: Examples of different cloud configurations causing OI. Photographs by Paola Russo.

as short term enhancements of global horizontal irradiance above clear-sky levels, are strongly linked to cloud edge effects and broken cloud conditions. Early observations in Spain demonstrated that irradiance of up to 130 % relative to clear-sky values can occur during partly cloudy situations due to forward scattering and reflections at cloud edges (Polo et al., 2012). At higher latitudes, similar events were reported (Zhao et al., 2014), finding that OI frequency increases in regions with rapidly evolving cloud fields, particularly during the summer months. Studies in Germany and the Netherlands further highlighted that mixed cloud layers and cumulus fields are especially prone to producing OI, with enhancements reaching values sufficient to stress photovoltaic components (Hoff and Perez, 2012; Lorenzo et al., 2011). More recently, a physical framework has been provided to explain these findings (Mol and Van Heerwaarden, 2025), identifying scattering mechanisms such as forward escape, downward escape, and side escape as the dominant processes behind observed over-irradiance. Collectively, these studies establish that OI is not a rare phenomenon but rather a recurrent feature in many climates, with significant implications for solar energy forecasting and PV system reliability.

Chapter 3 of this thesis will present a first statistical study (frequency, duration and magnitude) of over-irradiance events in Uruguay.

2.4. Surface and atmospheric information

Sites of study

In this work, ground data from two sites in Uruguay (Fig. 2.12) are considered. Salto is located in northern Uruguay and is characterised by low density rural settings and a sub-tropical inland climate. In contrast, Montevideo is a coastal city in southern Uruguay with moderate urban

2.4. Surface and atmospheric information

development and coastal influence. Both sites are 500 km apart, their coordinates and altitude are summarised in Table 2.2. Not every measurement is available in both sites, in Salto there



Figure 2.12: Satellite view of the sites considered in this work. Source: adapted from Google Earth.

is availability of G_h , G_{dh} , G_b , whereas in Montevideo there is availability of G_h , in both cases at 1 minute intervals. In both sites there are measurement campaigns of spectral irradiance $G_{b,\lambda}$, and in Salto there is a campaign of $G_{h,\lambda}$ and $G_{dh,\lambda}$. The Salto site is on the rooftop of the LES building and the instruments are class A, ventilated and receive periodic maintenance, including calibration every two years with traceability to the World Radiation Reference (WRR). The Montevideo site is located on the rooftop of Facultad de Ingeniería, where an AERONET station has been operating since 2020. The G_h measurements in Montevideo are maintained by LES and follow the same calibration protocols.

Table 2.2: Coordinates and altitude of the sites for ground measurements. Note $G_{h,\lambda}$ and $G_{dh,\lambda}$ are measured with the same instrument with a methodology described in Sec. 4.2.1.

Site	Lat. (°)	Long. (°)	Alt. (m.a.s.l.)	Broadband Meas.	Spectral Meas.	AERONET site
Salto	-31.2827	-57.9181	56	G_h , G_{dh} , G_b	$G_{h,\lambda}$, $G_{dh,\lambda}$, $G_{b,\lambda}$	No
Mvd.	-34.9182	-56.1665	58	G_h	$G_{b,\lambda}$	Yes

Ground based atmospheric information: AERONET

The AErosol RObotic NETwork (AERONET) from NASA ⁴, is a federation of ground based remote sensing aerosol networks, that is globally distributed in more than 400 sites in the world, in more than 80 countries, in several stations with the collaboration of various national agencies, institutes, universities and particular scientists.

It is mainly dedicated to providing estimates of atmospheric variables such as: AOD, precipitable water vapour w (cm) and radiance ($\text{W}/\text{m}^2/\text{sr}/\mu\text{m}$), among other sub products (Holben et al., 1998). Additional products such as Total Column Ozone or Nitrogen Dioxide are not measured but reported from other sources as the Ozone Monitoring Instrument (OMI⁵).



Figure 2.13: CIMEL sun photometer (extracted from: https://aeronet.gsfc.nasa.gov/new_web/photo_db_v5/Burjassot.html)

The network provides reliable and accurate long term atmospheric estimates of high quality, since they come from instruments that are periodically maintained and calibrated against the reference instruments from AERONET. Downloadable data have time variable frequencies, of around 15-20 minutes, since the CIMEL sun photometers take data in a variable time window and also the retrieval technique to estimate atmospheric parameters is performed under clear-sky conditions.

CIMEL Electronique sun photometers are classified as filter radiometers, and the instrument model over each site may vary. This instrument has a collimator tube and an automatic sun tracker incorporated. CIMEL is designed with a FOV of 1.2° , which is within the suggested angle for aerosol retrievals, of 2.5° (World Meteorological Organization, 2018). CIMEL measures beam

⁴<https://aeronet.gsfc.nasa.gov>

⁵<https://science.nasa.gov/mission/aura/omi>

spectral irradiance at narrow wavelength windows centred at specific wavelengths, typically 340, 380, 440, 500, 675, 870, 936 and 1020 nm.

The AOD product is obtained using retrieval algorithms developed by CIMEL/AERONET (Dubovik and King, 2000; Giles et al., 2019) specifically for the instrument. These algorithms are applied to $G_{b,\lambda}$ at each wavelength, and then AOD is obtained for each λ . To be applied, these algorithms need the calibration constants of the instrument, obtained by calibrating the sun photometers of the station (usually referred to as field sun photometers) against the reference sun photometers.

The calibration of the field sun photometers is performed every 6-12 months at Goddard Space Flight Center (GSFC), in Maryland, USA, where they also participate in an intercomparison which includes reference instruments. The reference instruments from GSFC are calibrated every 2-3 months at Mauna Loa Observatory, in Hawaii, at NASA facilities. The calibration method used is the Langley Plot Technique (Shaw, 1983) (described and used in Chapter 6). The calibration uncertainty of the field instruments is also analysed by AERONET. The field instruments are calibrated at GSFC, and intercompared before and after field deployment, against AERONET reference instruments (which are, besides, calibrated at Mauna Loa Observatory). In the traceability section of AERONET, it is published that the calibration uncertainty of field sun photometers dedicated to AOD retrievals is approximately 0.01 to 0.02 (Holben et al., 1998), wavelength dependent. Eck et al. (1999) also reported that the uncertainty in AOD retrievals obtained from CIMEL field instruments is approximately 0.01 in the visible and near-infrared spectral regions, mainly due to calibration uncertainty, and increases to approximately 0.02 in the ultraviolet wavelengths (340 and 380 nm). For the purpose of this work, the AOD from AERONET is considered as a reference value, with an estimated P95 uncertainty of ± 0.01 in the visible and near-infrared, and up to ± 0.02 in the ultraviolet region, and is used to assess the accuracy of the retrievals (Chapter 6) based on the EKO MS711 spectral measurements.

There are three levels of quality control of AOD estimated from CIMEL measurements. Level 1.0 means the data only has the initial manual inspection, applies temperature characterisations and considers absorption effects by NO_2 using OMI climatology data. Level 1.5 is based on level 1.0, and applies automatic cloud screening that considers the removal of optically thin cirrus contamination, preserves highly variable smoke, and quality control that include: the removal of sensor temperature induced errors, removal of AOD instants that corresponded to solar eclipses, removal of the impact of lens obstructions, removal of AOD instants with poor spectral dependence. Level 2.0 is based on level 1.5, with pre and post calibration applied and has minimal manual intervention. In this work, the data used in Chapters 4 and 6 is of level 2.0 or level 1.5, in that order of preference, depending on availability.

Satellite based atmospheric information: MODIS, OMI

MODIS stands for Moderate Resolution Imaging Spectroradiometer⁶. This instrument travels on board of the Terra and Aqua satellites from NASA (Fig. 2.14). As specific information, Terra passes daily over Uruguay around 9:15 AM (local time) and Aqua around 1:30 PM, thus Terra is more appropriate for morning estimates, and Aqua for afternoon estimates. Therefore, choosing the data from MODIS-AQUA or MODIS-TERRA depends on the specific project needs, as it will be mentioned in Section 4.2.2.

MODIS can measure Spectral Radiance ($\text{W}/\text{m}^2\mu\text{m sr}$) in 36 bands, discretised in varying bandwidths from wavelengths 620 nm to 14.385 μm . These wavelengths are useful for determining land and clouds properties, aerosols, ocean colour, phytoplankton, water vapour, cirrus clouds, among others (Salomonson et al., 1989). Its products are publicly available in NASA databases⁷, with a time resolution of 1 day approximately and are uploaded only a few days after the measurement has been performed by the instrument in the satellite. Its spatial resolution varies depending on the spectral band: in the wavelength range 620-876 nm its spatial resolution is of 250 m, from 459-2155 nm it is of 500 m, and in 405-14385 nm it is of 1000 m (specifications valid for the nadir⁸ direction).



Figure 2.14: Aqua Satellite from NASA <https://oceancolor.gsfc.nasa.gov/about/missions/aqua/>, which carries on board the MODIS Spectroradiometer.

The spectroradiometer on board the satellite measures the radiance reflected by the Earth after the radiation traverses the atmosphere, is reflected by the surface, exits the atmosphere, and finally reaches the satellite. From these measurements, atmospheric estimates are calculated

⁶<https://modis.gsfc.nasa.gov/about/specifications.php>

⁷<https://modis-gsfc-nasa-gov.translate.goog/data>

⁸Nadir is the point directly under the satellite, where the line of vision is exactly perpendicular to the Earth surface. Thus at nadir there is no geometrical distortion, the distance to the Earth is minimum and the spatial resolution is maximum.

using inversion algorithms that retrieve the desired parameter. Therefore, the beam has to pass twice through the atmosphere (with different optical paths). For this reason, the best accuracy is achievable with a sensor located at ground surface (where light only passes on time through the atmosphere). To illustrate this, Figure 2.15 shows how a passive satellite instrument would receive the light from the Sun in different cases, and how the optical path would be larger than if the instrument was located at ground level.

In this work, the atmospheric parameters aerosol optical depth and precipitable water vapour are used from MODIS-AQUA (from their original time intervals, interpolated to minute intervals) to model spectral irradiance. Extended information on the variables and procedures applied is presented in Section 4.2.

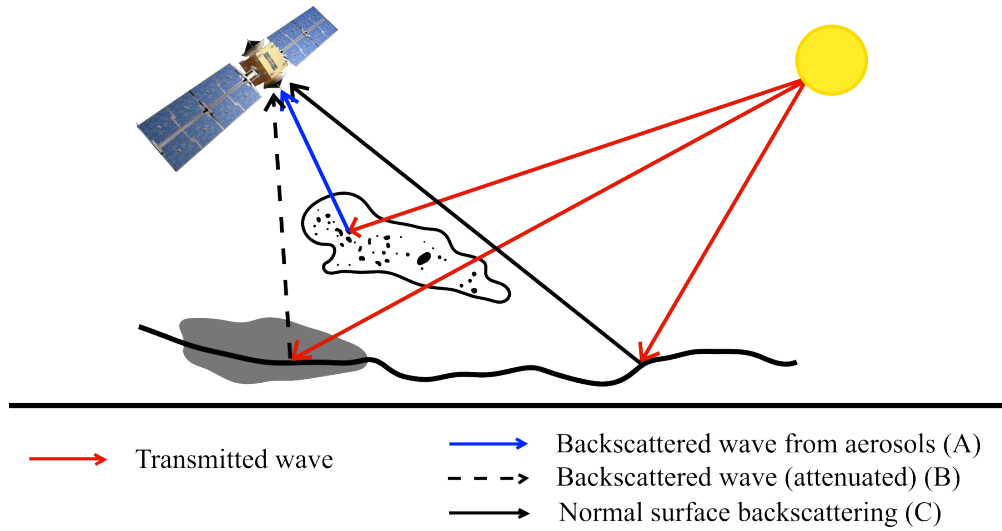


Figure 2.15: Satellite back scattering, adapted from (Danklmayer, 2008) for a passive instrument.

Another source of atmospheric information used in this thesis comes from the Ozone Monitoring Instrument (OMI, Levelt et al. (2006)), which is on board of the Aura satellite from NASA. This satellite passes daily over Uruguay at around 1.45 PM providing data with daily temporal resolution (Table 4.7). OMI measures solar backscattered radiation in the ultraviolet and visible range (270–500 nm) with a spectral resolution of approximately 0.45 to 0.63 nm. It has a width width of 2600 km, which allows it to cover all the Earth's surface once a day. OMI has been designed to estimate total column ozone and other air quality parameters such as nitrogen dioxide (NO_2), sulphur dioxide (SO_2) and aerosol properties. It has a high spatial resolution ($13 \times 24 \text{ km}^2$ at nadir⁹) which allows a detailed mapping of pollution sources.

⁹Notice nadir is the point directly under the satellite, where the line of vision is exactly perpendicular to the Earth surface. Thus at nadir there is no geometrical distortion, the distance to the Earth is

Reanalysis databases of atmospheric information: MERRA-2

Reanalysis datasets are physically-consistent reconstructions of the atmospheric state obtained by combining observational data with numerical weather models. They offer gap-free time series with global coverage across horizontal and vertical atmospheric layers. They are built combining climate models that solve physics laws using numerical methods, with large periods of observations from several sources such as: satellite estimates, meteorological ground stations, radio sondes, GPS, aircrafts, among others.

The estimates provided by reanalysis have uncertainties from different sources. Among them, there can be observational uncertainties (instrument errors, sampling errors, retrieval errors), model uncertainties (model physics, parametrizations, numerical errors), data assimilation uncertainties (bias correction, interpolation errors) and long term trends (satellite orbit drifts, instrument changes, reprocessing inconsistencies). Some of these sources are described in more detail in (Krueger et al., 2013; Parker, 2016; Thorne et al., 2017). It is important to consider them, to know the limitations and capabilities of these products.

Modern-Era Retrospective analysis for Research and Applications, Version 2 (MERRA-2), provided by NASA, is a satellite reanalysis database of free access ¹⁰, that covers the globe with a spatial resolution of $0.625 \times 0.5^\circ$. It was the first reanalysis database to incorporate space-based observations of aerosols in its algorithms, and consider their interactions with other physical processes in the climate system. Among the estimates for several atmospheric parameters provided since 1980, the ones used in this work are: Aerosol Optical Depth (unitless), Total Ozone Column (Dobson Units) and Precipitable Water vapour (originally in kg/m^2), all of them at regular intervals of 1 hour.

In this work, these parameters from MERRA-2 are used as inputs for Chapter 4 (modelling spectral irradiance), Chapter 5 (modelling broadband irradiance) and Chapter 6 (retrieval of AOD). A specific discussion of the uncertainty of the MERRA-2 estimates for the region will be presented in each chapter according to the specific parameters used. The high maintenance of MERRA-2, quality controls applied, accurate numerical algorithms, and extensive validation, make it a good option available to use for atmospheric inputs in the absence of more reliable ground-based data.

The accuracy of MERRA-2 estimates has been evaluated by comparison to ground measurements from AERONET sites. Recently, (Gueymard and Yang, 2020) performed a worldwide-scale validation of the aerosol products of MERRA-2 using 15 years of AERONET observations at 3 hour time intervals. For the region of interest of this work (Pampa Húmeda), Laguarda and Abal (2020) have performed a validation of MERRA-2 products: precipitable water vapour, aerosol optical depth at 550 nm and ozone, at 1-hour intervals, during the period 2008-2017, for three

minimum and the spatial resolution is maximum.

¹⁰For example: <https://giovanni.gsfc.nasa.gov/giovanni/>

AERONET sites in the region. They also discuss the sensitivity of clear-sky models to the uncertainties in each of these variables. The results of this evaluation are summarised in Table 2.3. The aerosol product AOD_{550} shows high dispersion, low correlation and a significant positive bias in the region. Water vapour has an acceptable dispersion with a significant positive bias.

Table 2.3: Validation of MERRA-2 atmospheric variables for the Pampa Húmeda region against three AERONET sites, hourly. See (Laguarda and Abal, 2020) for the details.

Metric	AOD_{550}	water vapour (cm)	Ångström exponent, α
rMBD (%)	17.5	7.1	-2.9
rRMSD (%)	33.4	11.2	26.8
Pearson correlation	0.72	0.95	0.36
# observations	40888	37024	38496
median	0.070	1.55	1.09

Several other reanalysis databases are in use, such as CAMS from Copernicus, Europe ¹¹, NCEP from NOAA, USA ¹², CRA-40 from CMA, China ¹³ among others. MERRA-2 has been compared against CAMS for AOD_{550} around the world (Gueymard and Yang, 2020) providing better results (MERRA-2: MBD=-0.011, RMSD=0.113, while CAMS: MBD=0.033, RMSD=0.268) and for this reason it has been chosen in this work.

When MERRA-2 is compared to direct satellite retrieval options, as MODIS, it offers some benefits. Among them, spatial and temporal continuity, data integration with previous bias correction and gap filling. All of these characteristics are relevant in this region of sparse measurement stations and sub-tropical climate.

Broadband solar irradiance measurements

Broadband measurements of G_h , G_{dh} and G_b are taken with specific instruments designed to have high accuracy, called pyranometers (G_h , G_{dh}) and pyrheliometers (G_b) Figure 2.16.

In the case of the Salto site, the instruments are mounted on a SOLYS2 Kipp & Zonen sun tracker, as shown in Figure 2.16, equipped with a precision positioning sensor device. Additionally, it has installed a shadow ball, which blocks a solid angle of 5° centred on the pyranometer measuring G_{dh} . Pyranometers are ventilated with warm air to keep them at constant temperature, which is relevant for their precision. On the other hand, the Kipp & Zonen pyrheliometers for G_b have a FOV of 5° .

¹¹<https://atmosphere.copernicus.eu/>

¹²<https://www.cpc.ncep.noaa.gov/>

¹³<https://data.cma.cn/>

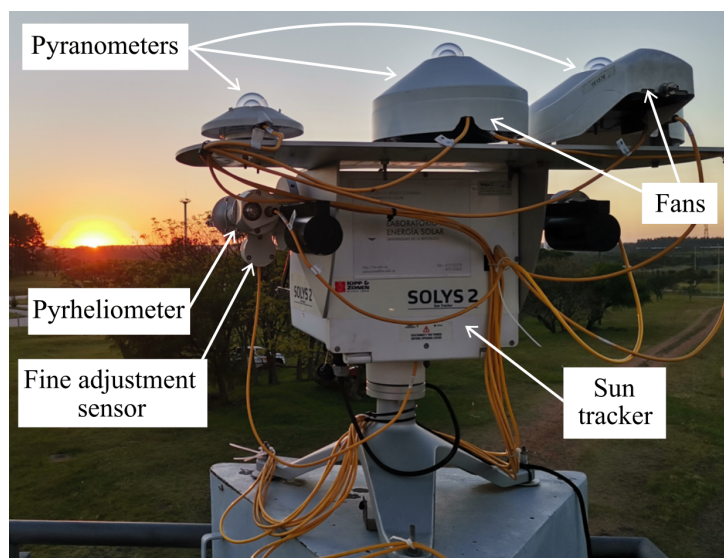


Figure 2.16: Broadband ground measurements in Salto site, with pyranometers and pyrhelimeters with fan ventilation, mounted on a sun tracker, which is pointing to the Sun at sunrise (East). Photograph by Paola Russo.

Measurements are periodically maintained by the LES staff, which includes weekly checks such as levelling, cleaning, alignment and periodic calibrations. For the case of pyranometers, they are calibrated every two years against a reference pyranometer from LES, using the Norm ISO 9847:2023(E) (2023) for the calibration of Pyranometers against a Reference Pyranometer. The reference pyranometer is recalibrated approximately every five years with the World Radiation Reference (WRR) at the World Radiation Center (WRC) in Davos, Switzerland. This process ensures the traceability of the measurements to the international radiation standard. This instrument, used as a secondary standard for Uruguay, remains stored in darkness and stable ambient conditions, and it is only taken to the exterior when a calibration is required. In the case of the reference pyrhelimeter, it was last calibrated during the International Pyrhelimeter comparison organised by the PMOD¹⁴ in Switzerland, on 2021/09/02. The traceability data, including models, series numbers, calibration factors, and active dates, is available in Table A.1.

The typical uncertainty of a class A ventilated and maintained pyranometer, such as Kipp&Zonen CMP10, is of 2 % under usual atmospheric conditions (ISO 9060:2018(E), 2018), and the typical uncertainty of a class A pyrhelimeter, such as a Kipp&Zonen CHP1, is less than 1 %, according to (ISO 9060:2018(E), 2018). The typical instruments installed in the measurement stations from LES are class A pyranometers and pyrhelimeters.

¹⁴Physikalisch-Meteorologisches Observatorium Davos

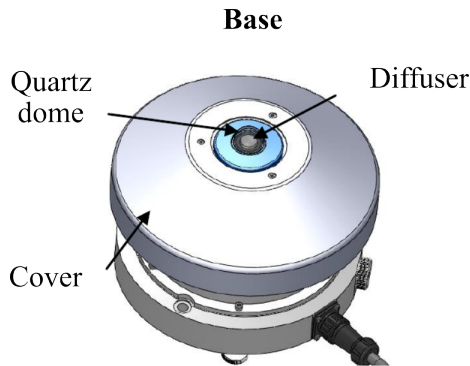
Spectral irradiance ground measurements

i) EKO MS711 N, Global

One of the instruments used in this work for spectral irradiance ground measurements is an EKO MS711 N designed for global measurements, and in this work is also used to measure the diffuse horizontal component (using a shadow ball and tracker). It is a grating spectroradiometer designed to measure continuously in outdoor conditions. Traceability information is available in Table A.2.

The instrument is located at the Salto station (Table 2.2). Measurements are recorded directly on the computer with the EKO Nami software and time labels are in UTC-3 (local time). The time is synchronised daily to the NIST time server¹⁵.

Figure 2.17 shows the spectroradiometer setting for measuring global spectral irradiance and a scheme of the basic parts of a global spectroradiometer. In Chapter 4 the use of this instrument is presented in the context of this work, including the measurement period, frequency, and methodology.



(a) Basic parts scheme.



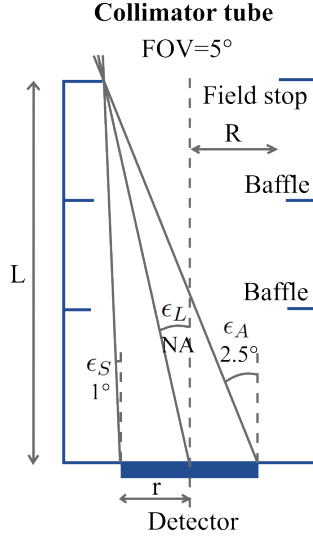
(b) Installed instrument.

Figure 2.17: Global spectroradiometer setting for measuring global, diffuse and beam and main components scheme, adapted from EKO (2016). Photograph by Paola Russo.

ii) EKO MS711, Beam (or Direct on normal incidence)

The EKO MS711 DNI is a collimated instrument designed to measure beam spectral irradiance. It consists of the same body as the EKO MS711 with the difference that it has no quartz dome and, instead, it has a collimator tube, with a quartz window on top. The collimator tube has

¹⁵time.nist.gov



(a) Collimator tube scheme.



(b) Installed instrument.

Figure 2.18: (a) EKO MS711 collimator tube scheme (adapted from EKO (2016)) and (b) the instrument is mounted on its precision solar tracker at Montevideo (photograph by Paola Russo).

a FOV of 5° , which coincides with the FOV of the CHP1 pyrhelimeter. Figure 2.18 (a) shows the relevant angles and FOV of the collimator tube. Similarly to the EKO for global, the EKO for beam is a spectroradiometer designed to measure continuously under outdoor conditions. More information on the instrument's working principle and technical details can be found in Appendix A.1. Traceability information is available in Table A.2. The EKO MS711 DNI is mounted on an EKO sun tracker system with an adjustment sensor for a precise position. The instrument was located for this work in Montevideo (Table 2.2), less than 20 meters away from the AERONET Montevideo station, on the same rooftop. Figure 2.18 (b) shows the instrument installed and measuring. Its measurements are recorded directly on the computer with the EKO WSDac software, using UTC-3 time, automatically updated every day using the NIST time server. In Chapter 6, direct normal spectral irradiance measurements from this instrument are used to retrieve atmospheric aerosol optical depth (AOD). Further details on the sampling frequency and measurement periods are precisely defined in the methodology of that chapter.

2.5. Performance metrics

Performance metrics quantify the performance of a model. Here, the mean bias deviation (MBD) and the root mean squared deviation (RMSD) between the estimate ($\hat{y}_i$) and the measurement (y_i) are used. Although this thesis focuses on comparisons against ground observations, other

reference sources, such as satellite-derived products or previously validated models, may also be considered for performance assessment.

For a time series of N estimates, in terms of residuals

$$\varepsilon_i = \hat{y}_i - y_i, \quad (2.25)$$

MBD and RMSD are defined as

$$\text{MBD} = \frac{1}{N} \sum_{i=1}^N \varepsilon_i \quad \text{and} \quad \text{RMSD} = \left[\frac{1}{N} \sum_{i=1}^N \varepsilon_i^2 \right]^{\frac{1}{2}}. \quad (2.26)$$

These metrics, have the same units as y and are frequently expressed in relative terms as a % of the average of the measurements $\langle y \rangle$. Then, $\text{rMBD} = 100 \times \text{MBD} / \langle y \rangle$ and $\text{rRMSD} = 100 \times \text{RMSD} / \langle y \rangle$ are their relative counterparts. Both provide complementary information, with RMSD measuring the dispersion of the estimated values relative to the measured or reference values Gueymard (2014). These metrics are suitable for evaluating broadband irradiance performance, because for each broadband component at a given instant there is a single measured value $\hat{y}$ to compare with the observation y . In contrast, for spectral irradiances, each instant provides an entire spectrum of values rather than a single measurement.

For spectral comparisons, a measure of the difference between the measured and estimated spectra is desired. The sum of residuals (or squared residuals to avoid cancellations) is an obvious alternative. Assuming that both spectra are discretised over L wavelength channels, the residuals at each wavelength $\lambda_j \in [\lambda_{j_{\min}}, \lambda_{j_{\max}}]$ are defined as

$$\varepsilon_{ij} = \hat{y}_i(\lambda_j) - y_i(\lambda_j), \quad (2.27)$$

where $i = 1 \dots N$ is associated to each spectral measurement (i.e time tag) and $j = 1 \dots L$ is associated to each wavelength in the range of interest. These residuals can be summed over all wavelengths and measurements to obtain the absolute spectral metrics,

$$\begin{aligned} \text{MBDs} &= \frac{1}{NL} \sum_{i=1}^N \sum_{j=1}^L \varepsilon_{ij}, \\ \text{RMSDs} &= \left[\frac{1}{NL} \sum_{i=1}^N \sum_{j=1}^L \varepsilon_{ij}^2 \right]^{\frac{1}{2}}. \end{aligned} \quad (2.28)$$

Even though these metrics are formally similar to those in Eq. 2.26, they describe different situations, since the sum over wavelengths is a global evaluation of the similarity between two spectra, so we use the suffix ‘s’ (spectral) to distinguish among them. These metrics can be

expressed in relative terms as a % of some reference spectral irradiance, usually the measured spectral irradiance averaged over spectra and wavelengths,

$$\langle y \rangle = \frac{1}{NL} \times \sum_{i=1}^N \sum_{j=1}^L y_i(\lambda_j), \quad (2.29)$$

where L is the number of discrete wavelength channels considered in the average.

An alternative, when spectral comparisons are made, is to use the relative residuals for each wavelength channel j ,

$$\epsilon_{ij} = \frac{\hat{y}_i(\lambda_j) - y_i(\lambda_j)}{y_i(\lambda_j)}, \quad (2.30)$$

where $i = 1 \dots N$ corresponds to each spectral measurement, as before. Then relative spectral metrics are obtained as

$$\begin{aligned} \text{rMBDs} &= 100 \times \frac{1}{NL} \sum_{i=1}^N \sum_{j=1}^L \epsilon_{ij}, \\ \text{rRMSDs} &= 100 \times \left[\frac{1}{NL} \sum_{i=1}^N \sum_{j=1}^L \epsilon_{ij}^2 \right]^{\frac{1}{2}}. \end{aligned} \quad (2.31)$$

An example of the use of these metrics can be found in Table 4.5. However, note that these relative metrics are expressed as a % of an unknown quantity. Furthermore, the use of relative residuals implies that those associated with lower spectral irradiances contribute more to the resulting metric than the same residual at a larger spectral irradiance, and these metrics can not handle channels with zero spectral irradiances. For these reasons, in this work, performance metrics are used based on absolute residuals, as defined in Eq. (2.28).

Chapter 3

Statistical analysis of over-irradiance events in Uruguay

This chapter is based on the work presented at the Solar World Congress (SWC, 2021), Virtual. The article is published as: Characterization of solar over-irradiance events in Uruguay. Russo, P., Laguarda, A., Abal, G. (2021). Proceedings SWC. Available at: doi: 10.18086/swc.2021.37.06, link: <https://proceedings.ises.org/conference/swc2021/papers/swc2021-0100-Russo.pdf>.

In (Russo et al., 2021), a first characterization of over irradiance (OI) events from broadband measurements in Uruguay is presented, introducing a statistical analysis of the events, focusing on their frequency, intensity, magnitude and duration. The study is based on a long term quality-controlled solar irradiance series registered at LES, in Salto (coordinates in Table 2.2), in the northern part of Uruguay, where the highest annual irradiation takes place.

Over-irradiance, as described in Section 2.3, results in an enhancement of the diffuse component of solar irradiance caused by particular short-lived cloud configurations, which leads to higher than expected global irradiance values. Usually, it does not affect beam irradiance.

3.1. Methodology

3.1.1. Data

The data used in this chapter consists of simultaneous records of G_h , G_{dh} and G_b irradiance registered at 1-minute intervals, in Salto (see coordinates in Sec. 2.4 and traceability details in Sec. A). The data set corresponds to five years (2016-2020) of continuous monitoring and has been subjected to adequate quality control procedures. The quality control consists of applying BSRN recommended filters (McArthur, 2005): 1-physically possible, 2-extremely rare, and 3-comparisons or closure consistency tests. Later, visual inspection is applied, to discard erroneous measurements. Additionally, only data with solar altitudes greater than 7° are considered, to

reduce the impact of cosine errors. Some OI events with lower solar altitudes may exist but they are associated with low G_h values and are not the focus of this analysis. Table 3.1 shows the number of samples of the initial diurnal data set, for complete records (G_h , G_{dh} and G_b) and that of the subsets that pass the quality filter and solar altitude.

Table 3.1: Filtered samples by quality control procedure (QC) and solar altitude. The percentages relative to the diurnal samples are shown in the last column.

diurnal samples	1,311,947	% of diurnal samples
samples that pass QC	962,430	disc. 26.6 %
diurnal samples with solar altitude $> 7^\circ$	947,015	total disc. 27.8 %
clear sky samples	397,622	selected 30.3 %

3.1.2. Over-irradiance detection

Several methods can be used to define and detect over irradiance events (OIE) (Castillejo-Cuberos and Escobar, 2020). Here, OIE are identified as those records for which the global horizontal irradiance (G_h) is above its corresponding clear-sky estimate ($G_{h,cs}$) by a certain threshold,

$$G_h > G_{h,cs} (1 + \xi) \quad (3.1)$$

where ξ is a positive dimensionless parameter to be determined and $G_{h,cs}$ is a clear-sky irradiance estimate, as described below. This definition is used for the automatic detection of OIE in the 1-minute G_h time series. Once the set of over-irradiance samples has been determined, its statistics are calculated. OIE are composed of several consecutive time intervals (minutes) in which G_h satisfies Eq. 3.1. If an OIE starts at t_1 and has a duration Δ (min), three characteristics are considered:

- i) duration (minutes): Δ ,
- ii) peak intensity I (maximum G_h during the event) in W/m^2 ,
- iii) magnitude (energy involved in the event): $M = \int_{t_1}^{t_1+\Delta} G_h(t) dt$, in J/m^2 (for time in s).

An exploratory study of the selected OI samples is carried out by analysing these quantifiable properties. The seasonal behaviour of these characteristics, as well as their occurrence distribution within a day, will be studied in what follows.

Clear-sky model validation

The choice of a clear-sky model is important for the identification of OIE from Eq. (3.1). Here the ESRA clear-sky model (Rigollier et al., 2000) is employed. This model uses the Linke Turbidity (TL, Ineichen and Perez (2002)) as its single atmospheric parameter and it has shown good accuracy over this region when used with locally derived cycles of daily mean TL (Laguarda and Abal, 2017; Laguarda et al., 2020).

As mentioned, this clear-sky model (with the local TL cycles) has been validated over the region in (Laguarda, 2021) at hourly timescale with clear sky irradiance measurements from several sites in Uruguay, including the one considered in the current work. The metrics used for the validation are rMBD and rRMSD, which have been defined in Section 2.5. The previous hourly validation over the site was performed using a standard random sampling and cross-validation process and shows a negative MBD of -0.2 %, RMSD of 2.9 %. For this study, a new validation was done using a 1-minute timescale. The results are shown in Table 3.2. The clear-sky samples were selected using the method described in (Reno and Hansen, 2016), imposing strict thresholds to avoid false positives and assure that true clear-sky samples are used.

In order to remove a potential dependence of the OI characterization results with the clear-sky model chosen, a standard linear site adaptation (Polo et al., 2016) was applied to the raw ESRA estimates. This procedure produces an unbiased clear-sky estimate and reduces the rRMSD to 3.5 % (see Table 3.2). This dispersion is similar to the uncertainty assigned to the measurements for 1-minute records. ESRA site-adapted will be used from here on as the clear-sky model.

Table 3.2: Performance of original and site adapted G_h estimates of ESRA clear sky model implemented for the work. % relative to the average of 397,622 clear-sky measurements = 624.6 W/m².

	Original (%)	Site adapted (%)
rMBD (%)	-3.8	0.0
rRMSD (%)	5.2	3.5

Determination of the threshold ξ

As stated in Eq. (3.1), a G_h measurement is considered OI when it exceeds the site-adapted clear-sky model by a coefficient $1 + \xi$, so the choice of the factor ξ is essential. Low values of ξ enhance the chance of incorrectly tagging clear-sky samples as OI (a false positive discrimination error). On the other hand, high ξ values will select only a subset of the real OI events (a false negative discrimination error).

For the determination of the optimum threshold, a statistical method is used, which consists of counting the fraction of selected clear-sky samples not tagged as OI, while varying the threshold ξ (as shown in Fig. 3.1). As the threshold increases, there are every time more clear-sky samples

that are not erroneously tagged as OI. But, there is a certain inflection point, where the curve stabilizes, this point is determined to be the optimum threshold. In this case, it is found to be $\xi = 0.105$, which corresponds to a 99.7 % of clear-sky samples not being tagged as OI. For this ξ , less than 1 % of the detected clear-sky samples are tagged as OI. It coincidentally corresponds to three standard deviations of the ESRA model uncertainty (P99 confidence level for a normal distribution of the residuals). Notice this is a restrictive definition if it is compared for instance to (Castillejo-Cuberos and Escobar, 2020), who uses $\xi = 0.05$, a value that would lead in this dataset to about 5 % of clear-sky samples tagged as OI, as shown in Fig. 3.1. Thus in this work, $\xi = 0.105$ is used in Eq. (3.1).

Selection of OI events

After selecting $\xi = 0.105$, a few samples are still erroneously identified as OI events. Thus, in a second iteration, the samples incorrectly selected as OI are removed using the clear-sky detection algorithm provided by PVlib (Holmgren et al., 2018) based on the criteria described in (Reno and Hansen, 2016). This criteria identifies 2.7 % of the OI pre-selected samples as clear-sky and these are removed from the OI group.

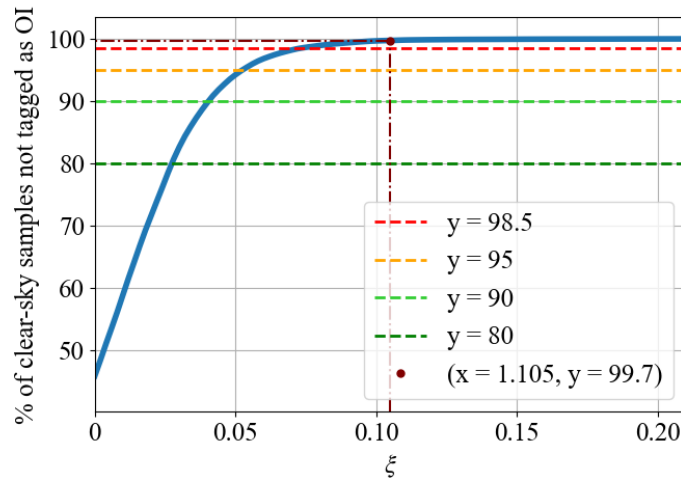


Figure 3.1: Fraction (%) of clear sky samples not tagged as OI versus ξ . Figure by Paola Russo.

The results of the previously described OI selection algorithm are summarized in a diffuse fraction (f_d) vs. clearness index (k_t) diagram, shown in Fig. 3.2. Notice that parameters f_d and k_t have been defined previously in Eq. (2.7) and Eq. (2.8), respectively. The figure shows all the measurements that passed the quality control procedure as grey dots. The records identified as OI events are shown in orange and the clear sky samples are coloured in light blue. Note that none of the OI samples are tagged as clear-sky since they are mutually exclusive categories.

As an example of the OI selection procedure, Fig. 3.3 shows the measured global (grey) and diffuse (green) together with the clear-sky estimate for the day 28/01/2020. The OI threshold is shown as a dashed maroon curve and the clear-sky estimate in light blue dots. Notice that the threshold must be large enough as to avoid erroneous identification of low sun (early morning, late afternoon) clear-sky samples as OI.

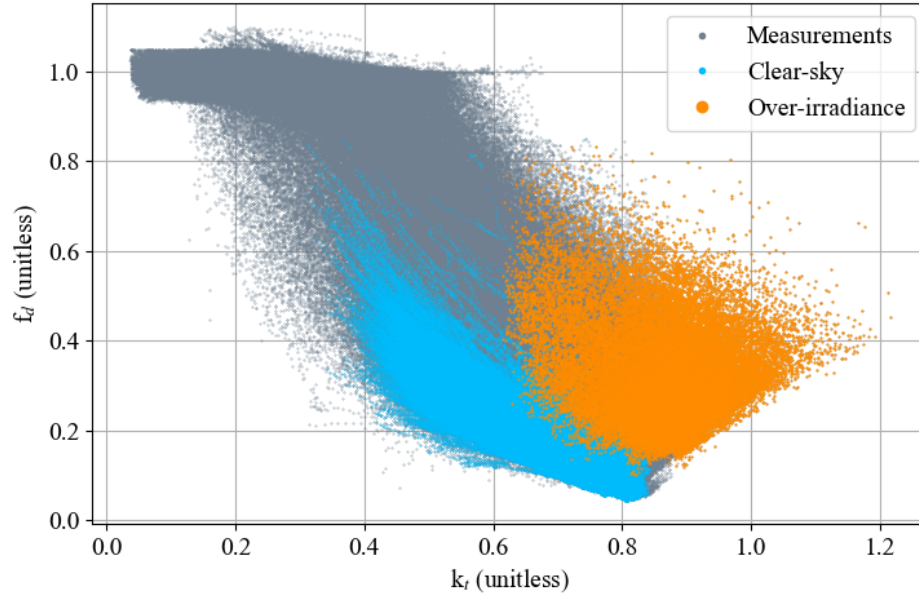


Figure 3.2: Diffuse fraction (f_d) vs clearness index (k_t) diagram for the quality-checked data (shown in grey). The light blue dots indicate clear sky samples and the orange dots identify OI samples. Figure by Paola Russo.

3.2. Statistical characterization of OIE

With the OI selection procedure presented, 4.2% of the 947,015 valid samples are selected as over-irradiance. As shown in Table 3.3, OI samples range from 3.0 to 4.9% of the data records from each year between 2016 and 2020. Although there is a percentage of samples which surpasses G_{0h} (defined in Eq. 2.5), these cases are rare and barely reach 0.2% of the total amount of samples each year. In order to evaluate if there is any seasonal dependence in the intensity of OI, the maximum values of OI registered by season-year are checked as a first approach. The results are shown in (Fig. 3.4). For each maximum value, the corresponding relative amount by which G_{0h} at the corresponding instant is exceeded, is indicated between brackets inside the bars (Fig. 3.4). For example, it is observed that the OI subset has a maximum G_h of 1601 W/m² during January 2017 (summer), which is 16.4% above G_{0h} . Additionally, the maximums per

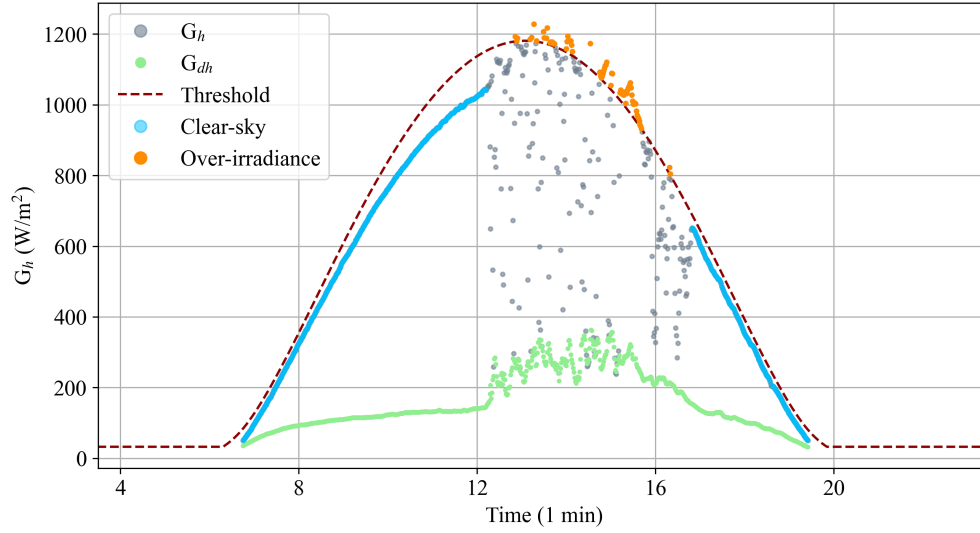


Figure 3.3: Example of OI detection on a time series (28/01/2020). Figure by Paola Russo.

Table 3.3: Seasonal characteristics of OI events.

Year	2016	2017	2018	2019	2020
Selected OI samples (%)	4.7	4.1	4.9	4.5	3.0
OI samples above horizontal TOA (%)	0.2	0.2	0.2	0.2	0.1
Valid data	178934	208030	173885	167910	218256

season-year (expressed in W/m^2) show certain dispersion, exceeding their corresponding G_{0h} by 2 % to 16 %. A similar range of values (between 1400 and 1691 W/m^2) has been reported in the literature (Castillejo-Cuberos and Escobar, 2020; de Andrade and Tiba, 2016; Gueymard, 2017; Inman et al., 2016).

Grouping consecutive samples with OI into OIE allows to analyse them according to their duration Δ and magnitude M (or energy flux involved). Figure 3.5 shows an histogram of the durations of OIE's. The orange dashed line corresponds to the P_{95} ¹ value. Most events fall below 10 minutes. Complementarily, Table 3.4 shows how the behaviour of Δ is quite stable across years, however it displays small seasonal variations, such that P_{95} has a value of 10 minutes in summer, 12 in autumn, 8 in winter and 9 in spring of 2016. On average, these P_{95} extreme events last less than 10 minutes.

¹Percentile 95 (P_{95}) is the value below which 95 % of the data falls. For a Normal distribution, P_{95} corresponds to values within approximately $\mu \pm 2\sigma$, where μ is the mean and σ is the standard deviation.

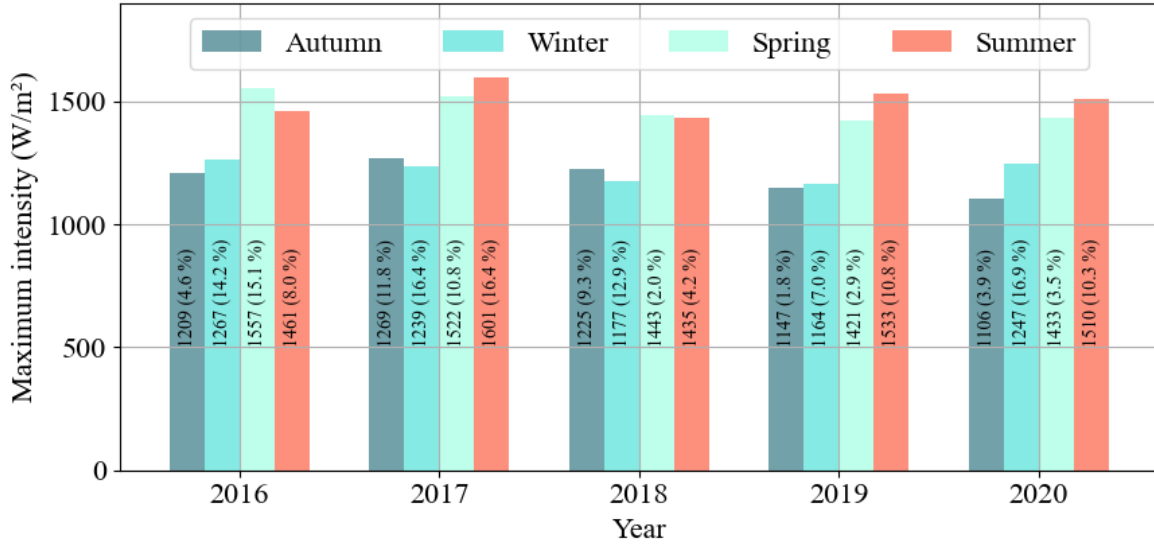


Figure 3.4: Maximum intensity of OIE (W/m^2). Figure by Paola Russo.

More information can also be extracted from Table 3.4, which shows that the amount of events is higher during summer, followed by autumn, spring and winter. Additionally, there is a significant variability in the total number of events across the years: for instance, there have been between 771 and 1185 events in summer. Furthermore, the largest events in duration typically occur in autumn, which could be explained by the greater presence of partial cloudiness. Seasonal histograms of M , defined in Section 3.1.2, are shown in Fig. 3.6, including the mean and P_{95} values in each case. Qualitatively speaking, the histograms are similar across all seasons. From a quantitative point of view, the most energetic events (as measured by the average and P_{95} values) occur during summer. In autumn and spring they are moderate and similar to each other, and in winter they are the least energetic. As a reference, a 5 minute OIE at a constant irradiance of $1000 \text{ W}/\text{m}^2$ represents a magnitude of $300 \text{ kJ}/\text{m}^2$.

The seasonal peak intensity (PI) distributions of the OIEs, along with their mean and P_{95} values, are shown in Fig 3.7. The histograms show that PI is differently distributed throughout the year. The highest intensity peaks occur during spring and summer, with values greater than $900 \text{ W}/\text{m}^2$ and P_{95} of $1300 \text{ W}/\text{m}^2$. During autumn and winter intensities decrease to similar values of approximately $660 \text{ W}/\text{m}^2$ (mean) and $1030 \text{ W}/\text{m}^2$ (P_{95}).

Finally, in addition to the seasonal dependence, it is also analyzed at what time of the day are OIE's most frequent. For this, OIE's occurrences are plotted on a solar diagram (solar altitude vs. solar azimuth angles) in Fig. 3.8, where brighter colours indicate more occurrences. For winter and autumn (lower region of the diagram), the OIE's occur mainly around noon (azimuth angles

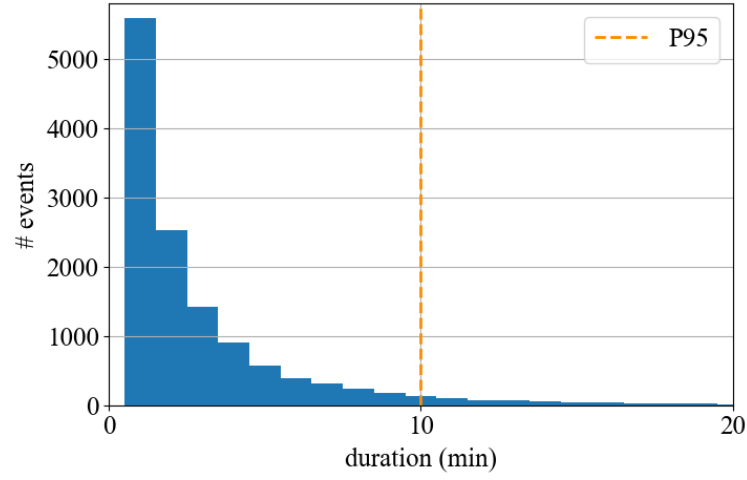


Figure 3.5: OIE duration, Δ (min). The P_{95} duration is 10 minutes. Figure by Paola Russo.

Table 3.4: Number of OIE and its P_{95} duration by season and year. The year in which each variable records a maximum is highlighted in gray.

	Year	2016	2017	2018	2019	2020
Number of OIE	summer	771	1185	836	1133	800
	autumn	649	828	685	630	464
	winter	439	301	497	216	260
	spring	927	629	640	445	492
Δ at P_{95} (minutes)	summer	10	11	11	10	10
	autumn	12	10	13	12	11
	winter	8	7	8	9	10
	spring	9	9	9	8	10

near 0°). In the upper region, which is related to spring and summer, the occurrences are more smoothly distributed with greater presence during mornings and afternoons (that is azimuth angles greater than 50° or smaller than -50° respectively). The behaviour is almost symmetrical.

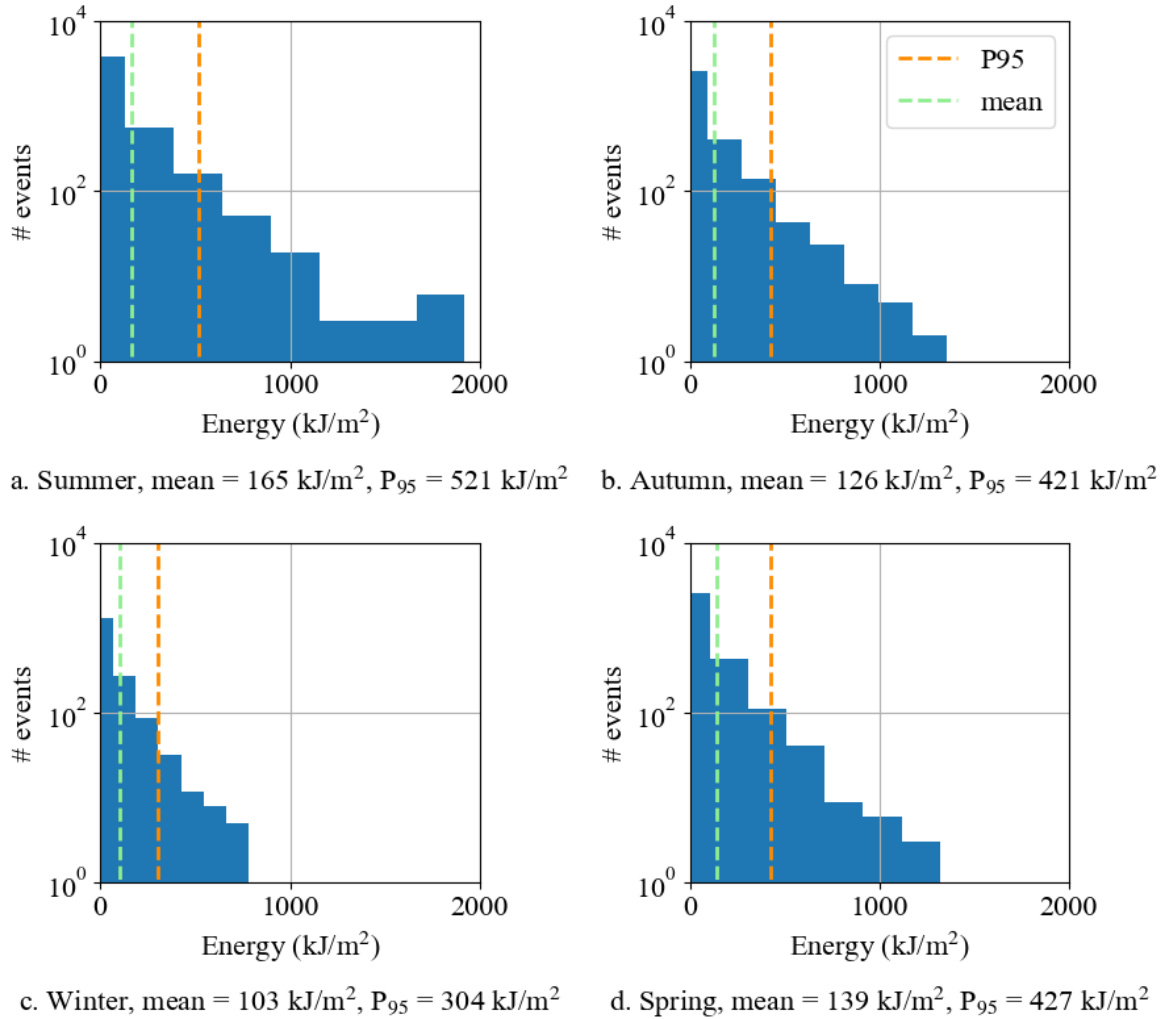


Figure 3.6: Histograms of Magnitude of OIE, classified by seasons. Energy Magnitude, Mean and P₉₅ are expressed in kJ/m². The vertical axis is in logarithmic scale. Figure by Paola Russo.

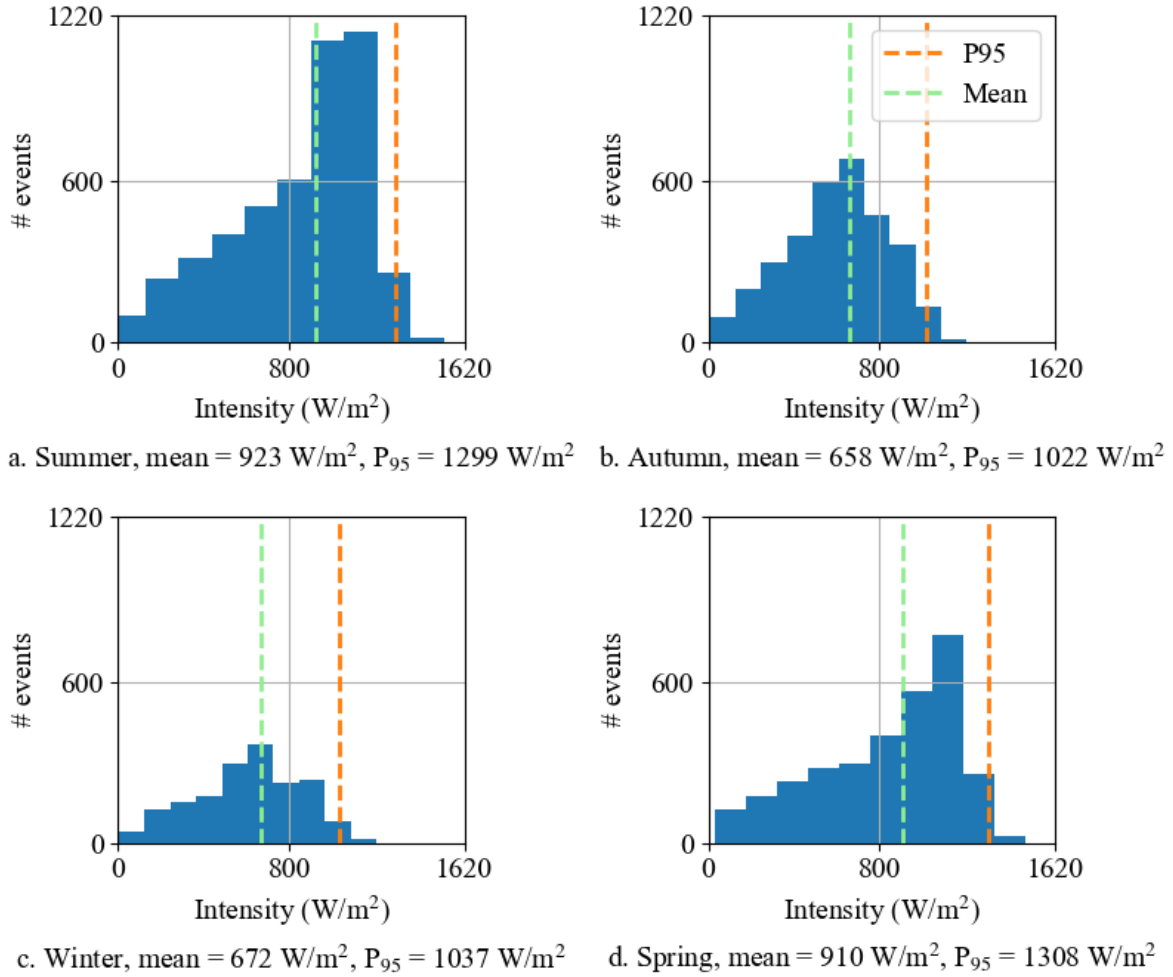


Figure 3.7: Histograms of peak intensity (in W/m^2) of OIE, classified by seasons. Figure by Paola Russo.

3.3. Conclusions

A first statistical analysis of solar over-irradiance events was carried out using 5 years of 1-minute data for a site in Uruguay, which is representative of the Pampa Húmeda region. The threshold method proposed for deciding whether a sample is considered of over-irradiance (OI) or not, consisted in determining if its G_h surpassed a threshold locally adjusted clear-sky model multiplied by a factor $(1 + \xi)$. The best value for this parameter was obtained from the data.

Over-irradiance records are frequent throughout the year, and represent an average of 4.3 % of the recorded data. Their typical duration is usually less than 10 minutes (P_{95}), being a little longer in autumn.

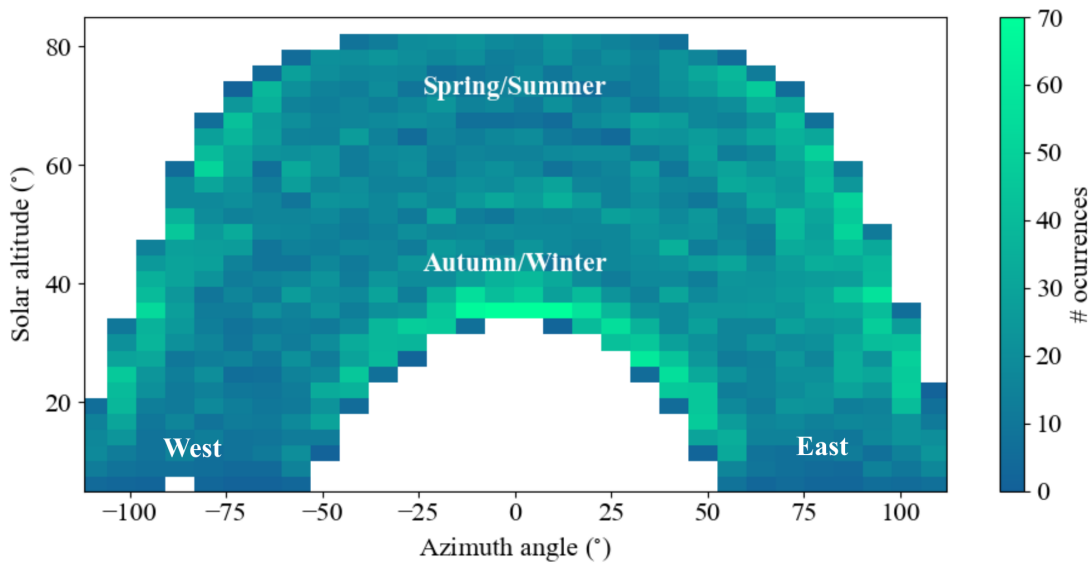


Figure 3.8: Over-irradiance occurrences in a solar diagram. Colours indicate the number of occurrences. Figure by Paola Russo.

Their average magnitudes followed a clear seasonal trend, occurring the most energetic events in summer (mean of 165 kJ/m^2) and the least energetic events in winter (103 kJ/m^2). During the rest of the year, autumn and spring, they showed intermediate magnitudes (130 kJ/m^2). On the other hand, their mean peak intensity showed a different pattern, it was around 900 W/m^2 during summer and spring, and lower during autumn and winter (around 650 W/m^2). Additionally, the maximum peak intensity (P_{95}) was slightly greater in spring than in summer (1308 and 1299 W/m^2 , respectively) and greater in winter than in autumn (1037 and 1022 W/m^2 , respectively) however these differences were hardly significant.

Focusing on the daily distribution of OIE's, interesting results were obtained. The study showed that during winter and autumn they occur mainly around solar noon and in the early afternoon. However, a shift happens in spring and summer, when OIE's start happening mostly at lower solar altitudes, meaning in the mornings and afternoons.

Regarding the type of clouds that could be causing this events, no sky camera was analysed, and the distribution of k_t or k_d values associated to OIEs was not investigated in this first approach. These aspects are left for future work. Previous studies have shown that broken cumulus clouds with pronounced edges are the dominant drivers of OI, as they enhance solar irradiance through forward scattering and lensing effects at cloud boundaries (Gueymard, 2017; Nann and Riordan, 1991). The cloud classification proposed by Mol and Van Heerwaarden (2025) further supports this interpretation, identifying cumulus-type clouds, particularly in transitional convective regimes, as the primary generators of short-lived irradiance spikes. OIEs were found to occur more frequently during the morning and afternoon hours, which may be associated with the presence of convective cloud fields (Cairns, 1995). While the decreased occurrence of events during summer midday could be associated to increased solar heating around local noon, which modifies boundary-layer turbulence and cloud evolution (Stull, 1988).

Overall, the presented methodology has a good balance between the amount of information it provides and its ease of implementation. In this regard, it has significant application potential, as it only requires G_h measurements at 1-minute intervals, the most commonly recorded variable at radiometric stations. Due to these reasons, it might be implemented in photovoltaic plants to design their components to mitigate OI effects. It could also be applied by on-grid or off-grid civil users to enhance energy management strategies and improve the grid system reliability. Additionally, the comprehensive statistical analysis presented here could be scaled to a broader region or extended to larger time datasets to assess spatial and temporal variability for climatic applications.

For future work, complementary to the statistical approach presented to study over-irradiance, a physical perspective could provide deeper insights into the mechanisms driving these events. This could involve applying radiative transfer models to simulate OI conditions at high spatial resolutions under varying atmospheric scenarios, such as the presence of clouds or aerosols. Additionally, analyzing how OI affects the local surface energy balance may provide insights into its thermodynamic implications and potential inputs into the atmosphere. Furthermore, studying how aerosol concentration or surface reflectivity interact to amplify or mitigate OIE's would further enhance the understanding of the phenomenon from a physical perspective.

Chapter 4

SMARTS clear-sky spectral irradiance model

In the absence of clouds, spectral irradiance can be modelled from a physical point of view where an incident extraterrestrial solar flux is assumed and several scattering and absorption processes that take place in the (cloudless) atmosphere are considered. Advanced radiative transfer models, such as DISORT-libRadtran (Emde et al., 2016), can account accurately for most relevant radiation-atmosphere interactions, but they are computer-intensive. Even when there are simplified algorithms that solve radiative transfer equations which are more computer efficient, such as MOMO (Doppler, 2013), they still require detailed atmospheric input data and assumptions of the vertical structure of the atmosphere, aerosol and cloud properties. For these reasons, radiative transfer models may be impractical for some applications. On the other hand, simplified models, which parameterize most radiation-atmosphere interaction processes using fast algorithms, can produce accurate clear-sky estimates of spectral solar irradiance at ground level, using a simplified description of the atmosphere.

Among these, SMARTS (Simple Model of the Atmospheric Radiative Transfer of Sunshine) (Gueymard, 1995, 2001, 2018, 2019) has been developed to achieve a good balance between accuracy, flexibility and simplicity, and has been used worldwide in a wide range of applications, as discussed in Gueymard (2019). However, despite its extensive use, there are relatively few quantitative evaluations of SMARTS, and in particular, very few conducted in the region of interest (Pampa Húmeda, Uruguay). For this reason, this chapter presents an assessment of several outputs from SMARTS, evaluating the accuracy of this spectral model against ground based data. Section 4.1 presents the structure and details of SMARTS, to enable a comprehensive understanding of the model, Section 4.2 describes the methodology applied and Section 4.3 discusses the results obtained.

4.1. SMARTS description

SMARTS (Gueymard, 1995, 2001, 2018, 2019) was originally developed as an improved version of the FORTRAN-based model SPECTRAL2, which was originally created by the National Renewable Energy Laboratory (NREL, USA). Code for SMARTS (versions 2.9.2 and 2.9.5) is free for civil research or educational purposes and can be downloaded from the Solar Consulting Services site¹. It is a parametrized physical model that allows to estimate the spectral irradiance that arrives to the ground surface (usually horizontal) $G_{h,\lambda}$ and its components $G_{dh,\lambda}$, $G_{b,\lambda}$ in the range 280 – 4000 nm with resolutions between 0.5 (UV range) and 5 nm (NIR range). Other outputs include the transmittance T_λ of different atmospheric constituents, the spectral irradiance that a spectroradiometer would measure at ground level in cloudless conditions, among other magnitudes. The last version available to the general public at the beginning of this work is 2.9.5, and it is the version used in this work.

The model estimates $G_{b,\lambda}$, based on the physical Law of Exponential Attenuation from Lambert (Eq. 2.20). As a central hypothesis, SMARTS assumes that the attenuation effects of each atmospheric component are independent from each other. This assumption allows the transmittance T_λ to be expressed as a product of individual transmittances corresponding to each attenuation process, $T_{i\lambda}$, as shown in Eq. 4.1. The main components causing attenuation of the solar beam are listed in Table 4.1. The subindex λ is included to emphasize that these are spectrally selective processes.

$$G_{b,\lambda} = G_{0h,\lambda} T_{r\lambda} T_{o\lambda} T_{n\lambda} T_{g\lambda} T_{w\lambda} T_{a\lambda}. \quad (4.1)$$

In the interaction of photons with a real atmosphere, this is a simplification, but it is a reasonable one under the certain conditions (Gueymard, 1995). These conditions can be summarized as follows:

- i) spectral domains must be sufficiently separated. This means that each gas must dominate in its own spectral window, so that the overlap between absorption features is negligible and the model can safely treat each absorber as independent.
- ii) Scattering must be mainly single scattering, this means the photon must be scattered only once before it reaches the ground (for example, by one air molecule or one aerosol particle), as happens usually in low turbidity and relatively clear skies. This assures that the probability of scattering interacting in a complicated way with absorption (for example a photon being scattered and then absorbed by water vapour) is small. It also assures that saying that each process (for example, scattering, ozone absorption) is independent from each other is a good approximation.

¹<https://solarconsultingservices.com/smarts.php>

- iii) The atmosphere is optically thin, so that Lambert Law is applicable, because each photon interacts independently and the probability of interaction is proportional to the path length and the absorber concentration.

Table 4.1: Atmospheric processes that cause attenuation considered by SMARTS.

	Process
r	Rayleigh scattering
o	ozone
n	nitrogen dioxide
g	mixed gases
w	water vapour
a	aerosol extinction

SMARTS also estimates $G_{dh,\lambda}$ using a model that will be described below, and later $G_{h,\lambda}$, is calculated from the closure relation, Eq. (2.6).

Relative optical air mass

The relative optical air mass (m), Eq. (2.11), is calculated for each component using the general parametrization shown in Eq. (4.2),

$$m_i = \left[\cos \theta_z + a_{i1} \theta_z^{a_{i2}} (a_{i3} - \theta_z)^{a_{i4}} \right]^{-1}, \quad (4.2)$$

where the sub indexes i from m_i correspond to the processes described in Table 4.1, and θ_z is in degrees. Coefficients a_{i1} to a_{i4} are tabulated for each component in Table B.3 from Appendix B.9.

Reference atmosphere

The reference atmosphere provides a standardized representation of the vertical profile for temperature, pressure and concentration of several gases, thus it is required to be specified before the modelling starts. The U.S. Standard Atmosphere (USSA) of 1976 is one option, but there are several alternative profiles, five of them are from the MODTRAN model: Mid-Latitude Summer (MLS), Mid-Latitude Winter (MLW), Sub-Arctic Summer(SAS), Sub-Arctic Winter (SAW) and Tropical (TRO) profile. Four additional options are included in SMARTS: Sub-Tropical Summer (STS), Sub-Tropical Winter (STW), Arctic Summer (AS) and Arctic Winter (AW), (Myers and Gueymard, 2004).

In this work, the reference atmospheres that will be used are SMARTS STS and STW because the study is focused on a sub tropical site. For this purpose, when data corresponds to summer and spring, STS will be used and when it corresponds to winter and autumn, STW will be used.

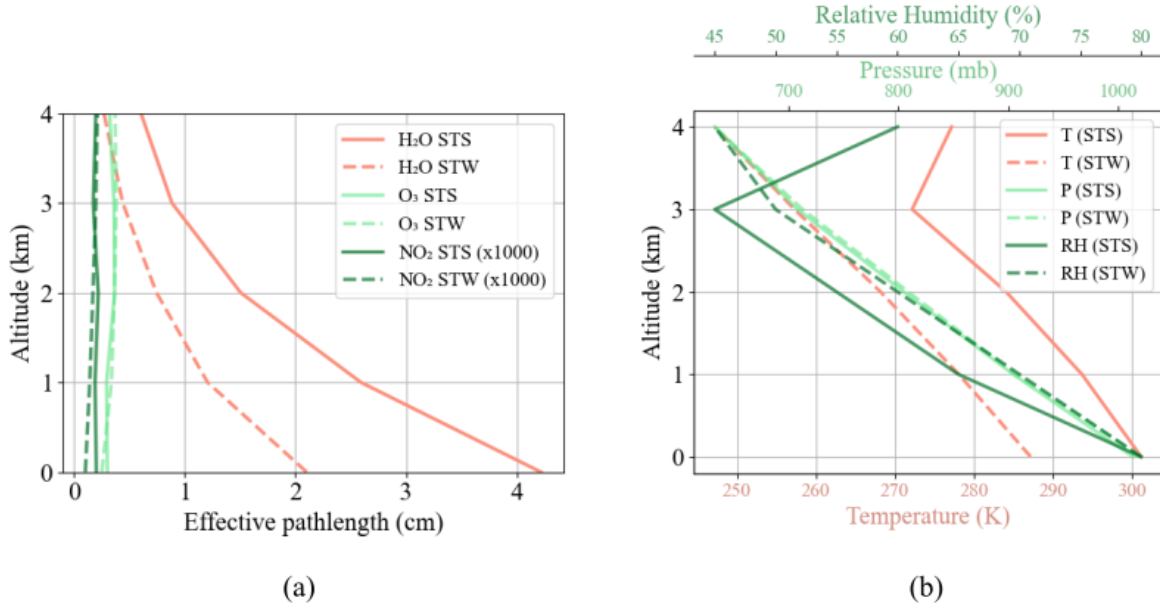


Figure 4.1: For different reference atmospheres: (a) effective path-lengths, (b) vertical profiles of relative humidity, atmospheric pressure and temperature. Figure by Paola Russo.

Figure 4.1 shows the profiles of density (as effective pathlength), temperature (T, K), pressure (P, hPa) and relative humidity (RH, %) depending on the altitude (km), for the reference atmospheres STS and STW. Complementarily, Table B.4 shows a summary of the values tabulated for this atmospheres, extracted from (Gueymard, 1995). Observe how, as altitude increases, pressure decrease due to the thinning of the atmosphere and reduced air density at higher elevations. Relative humidity also tends to decrease with altitude, reflecting the lower water vapor capacity of colder air. In the STS profile, temperatures are generally higher than in STW, consistent with seasonal solar heating. Pressure profiles are similar but slightly higher in STW near the surface. In STS there is a inversion in the slope of T and RH at around 3 km (altitude of the limit layer). This is because in summer the ground surface is strongly heated, creating a high limit layer (3 km). Above it, the anticyclonic movement compresses air and heats it, more than in the below layers. In winter this does not happen, because the ground surface heating is not so strong, instead, there is a weaker inversion, due to surface cooling during the night. These vertical distributions are fundamental for understanding radiative transfer, cloud formation, and atmospheric stability. Regarding the effective path lengths, H₂O decreases sharply with altitude because water vapor is primarily confined to the lower troposphere, where temperatures are higher and the air can hold more moisture. It is lower in winter (STW) than in summer (STS) due to reduced evaporation and colder temperatures. On the other hand, O₃ shows relatively constant or slightly increasing values with altitude, consistent with its production from photo

chemical reactions that locate in the upper troposphere and stratosphere. NO₂ remains stable with altitude and at low concentrations, reflecting its origin as a near-surface pollutant with limited vertical transport. The slightly higher NO₂ values in STS near the surface may result from enhanced emissions or slower oxidation under warmer conditions. These patterns reflect the distinct sources and typical transport mechanisms governing each gas in the atmospheric column.

4.1.1. Beam spectral irradiance

SMARTS relies on several parametrizations for the attenuation processes in a cloudless atmosphere. The expressions and parametrizations described in this subsection are from (Gueymard, 1995). They are presented here for completeness and to provide an overview of how the model works, with the aim of understanding its main structure, however they do not provide exhaustive detail, since this has already been thoroughly described in SMARTS documentation.

Rayleigh transmittance

Even though Rayleigh theory establishes that the Rayleigh optical depth is proportional to the inverse of λ^4 (Section 2.2), this represents a first order approximation. SMARTS uses the empirical parametrization of (Kerker, 1969; McCartney, 1976) to compute $\tau_{r\lambda}$:

$$\tau_{r\lambda} = P / [P_0 (a_1 \lambda^4 + a_2 \lambda^2 + a_3 + a_4 \lambda^{-2})], \quad (4.3)$$

where P is the atmospheric site pressure (hPa), P₀ is the standard pressure 1013.25 hPa and P/P₀ is the pressure ratio, a dimensionless factor. The factors a_i are: $a_1 = 117.2594 \mu\text{m}^{-4}$, $a_2 = -1.3215 \mu\text{m}^{-2}$, $a_3 = 3.2074 \times 10^{-4}$ and $a_4 = -7.6842 \times 10^5 \mu\text{m}^2$.

Ozone transmittance

The total ozone optical depth is parameterized as

$$\tau_{o\lambda} = u_o A_{o\lambda}. \quad (4.4)$$

It is calculated using the ozone total path-length, u_o (atm-cm, described in Appendix B.11), which is an input parameter from the user, and the Spectral Absorption Coefficient ($A_{o\lambda}$). The path length is related to how much gas is present along the path, a smaller value means there is less of the certain gas and a greater value means there is more of that gas. In Figure 4.2, the transmittances are represented for different path lengths, for each gas. For example, a thin atmosphere with a small O₃ path length (0.2 atm-cm) absorbs little, and its transmittance is close to 1. But a thick atmosphere with a large O₃ path length (2.5 atm-cm) has a strong absorption, and less irradiance is transmitted (transmittance decreases to around 0.7). It is also observed in Figure 4.2, that the ozone transmittance curve shows significant attenuation in

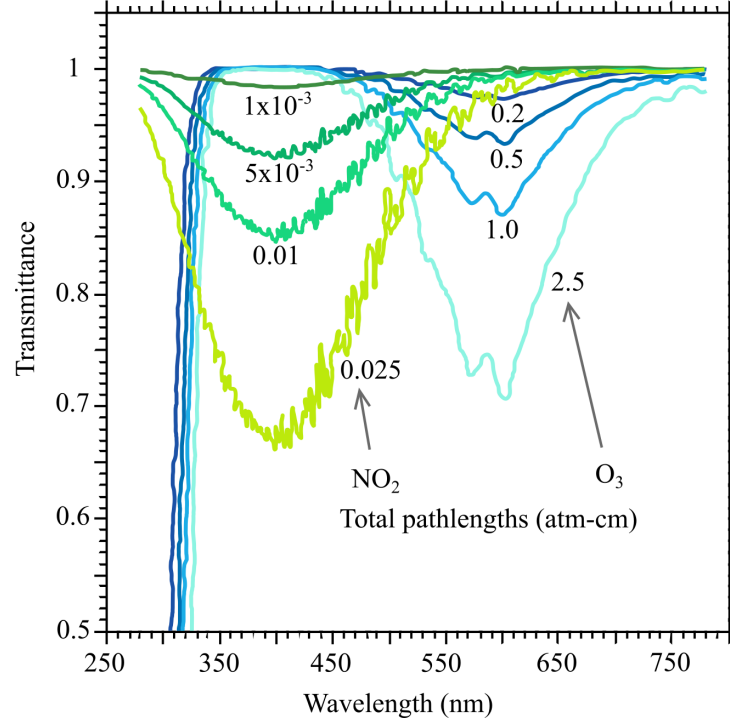


Figure 4.2: SMARTS transmittances of Ozone (shades of blue) and Nitrogen Dioxide (shades of greens), for several optical path-lengths, $u_{o,i}$ and $u_{n,i}$ (such as 0.01, 1.0 and so on). Adapted from Gueymard (1995).

specific spectral regions where ozone molecules absorb incoming solar radiation. This behaviour is particularly evident in the UV and visible parts of the spectrum. The decreases correspond to the well-known absorption bands of ozone: Hartley band (Hartley, 1880) (approximately between 200–310 nm), where ozone strongly absorbs UV radiation, resulting in transmittance values close to zero, Huggins band (Huggins, 1890) (around 310–350 nm), where absorption is weaker but still noticeable and Chappuis band (Chappuis, 1880) (450–750 nm), which causes a mild valley in the visible spectrum, although the absorption is relatively weaker compared to the UV bands. Additionally to the strong absorption in the UV region, and the moderate absorption in the visible region, ozone has a small absorption in the near infrared region. This complex spectral selectivity is represented in the model by the parameter $A_{o\lambda}$, which depends on the ozone effective temperature, T_{eo} (which mainly depends on the vertical distribution of ozone and the temperature profile of the atmosphere):

$$A_{o\lambda}(T_{eo}) = \max \{0, A_{o\lambda}(T_{ro}) + c_1(T_{eo} - T_{ro}) + c_2(T_{eo} + T_{ro})^2\}, \quad (4.5)$$

where: T_{ro} refers to the reference laboratory temperature of ozone, in this case, $T_{ro} = 228$ K, and the coefficients: c_1 , c_2 , are parametrizations depending on the wavelength range, see Gueymard

(1995) for specific values. As an example, Appendix B.11 shows how the ozone transmittance is computed with different parametric expressions depending on the wavelength range.

Nitrogen dioxide transmittance

Nitrogen Dioxide absorption is calculated as shown in Eq. (4.6)

$$\tau_{n\lambda} = u_n A_{n\lambda}, \quad (4.6)$$

where $A_{n\lambda}$ is the absorption coefficient for NO_2 , and u_n is the total path-length (atm-cm, described in Appendix B.11). Figure 4.2 shows the nitrogen dioxide transmittance for different total path lengths. The plot shows strong spectral selectivity with specific spectral regions, where NO_2 molecules selectively absorb incoming solar radiation. This behaviour is mostly apparent in the UV, visible and NIR regions of the spectrum. Such attenuation correspond to NO_2 absorption bands that have been previously studied by different authors. Among them, the Hartley band (Hartley, 1889) (approximately between 400–450 nm), where NO_2 absorbs strongly, leading to significant attenuation and a steep drop in transmittance, the Matsumoto-Yamanaka absorption feature (Matsumoto and Yamanaka, 1992) (around 430–460 nm), which contributes to a moderate dip in the visible spectrum, and the Huggins band (Huggins, 1939) (near 310–390 nm), where NO_2 absorbs more weakly but still noticeably, especially in the UV region. These dips reflect the specific absorption characteristics of NO_2 across the solar spectrum. Further than 600 nm there is no substantial absorption produced by NO_2 and the transmittance remains flat. Considering this, $A_{n\lambda}$ is modelled as a function of the effective temperature, T_{en} :

$$A_{n\lambda}(T_{en}) = \max \left\{ 0, A_{n\lambda}(T_{rn}) \left[1 + (T_{en} - T_{rn}) \sum_{i=0}^{i=5} f_i \lambda^i \right] \right\}, \quad (4.7)$$

where: $T_{rn} = 243.2$ K is the reference temperature for nitrogen, and f_i are empirical coefficients specific for the $\lambda < 625$ nm and $\lambda \geq 625$ nm regions (see Table B.5 from Appendix B.11 for details).

Uniformly mixed gas absorption

Gaseous absorption is also modelled with a parameterized extinction equation (Eq. 4.8) similar to the ones presented for ozone and nitrogen dioxide, assuming the gas optical mass as $m_g = m_R$, a spectral absorption coefficient, $A_{g\lambda}$, an altitude-dependent gaseous scaled path length, u_g , and a wavelength dependant exponent, a . Full expressions for $A_{g\lambda}$, u_g and a are available in (Gueymard, 1995).

$$T_{g\lambda} = e^{-(m_g u_g A_{g\lambda})^a}. \quad (4.8)$$

Water vapour absorption transmittance

Water vapour is the most important absorbent in the near infrared (NIR) spectrum. Figure 4.3 shows how the transmittance is reduced at the specific wavelengths where water vapour attenuates the irradiance. The strongest absorption bands are observed around the 940 nm and 1130 nm wavelengths. Water vapour transmittance throughout the whole spectrum has been thoroughly studied by previous authors, among them (Rothman et al., 1996) for HITRAN and (Clough et al., 2005).

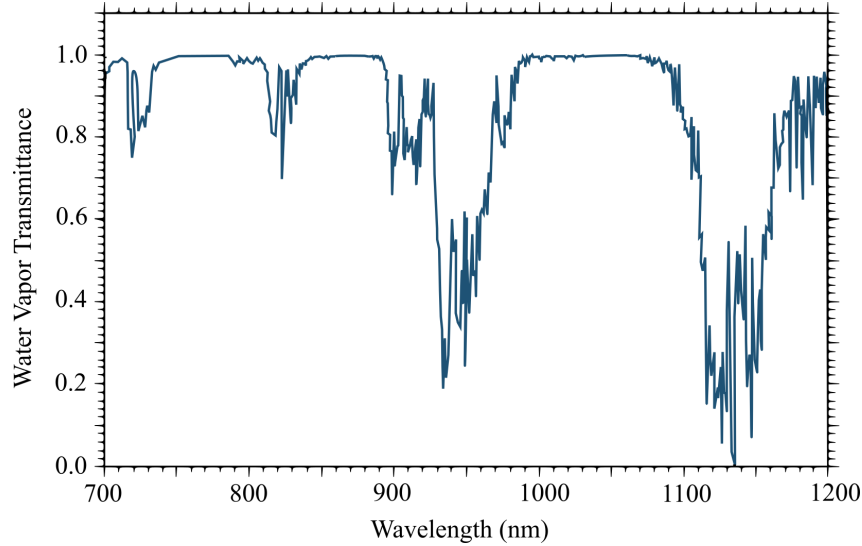


Figure 4.3: Water vapour transmittance modelled by SMARTS using $w = 1.419$ cm, the U.S. Standard Atmosphere and $m = 1.5$. Adapted from Gueymard (1995).

As it has been mentioned, SMARTS approximates the attenuation of solar radiation due to different components using a semi-empirical expression based on the Lambert Law, Eq. 2.20. This law relates transmittance to the exponential of the air mass and optical depth τ_λ , assuming a linear dependence between the attenuation and the amount of absorber. However, in the case of water vapour, absorption is highly nonlinear due to the dense distribution of rotational-vibrational lines and their broadening under varying pressure and temperature conditions.

To better capture this complexity, SMARTS replaces the simple transmittance (linear dependence in the exponent) with a nonlinear formulation

$$T_{w\lambda} = e^{-[(m_w w)^{1.05} (f_w)^n B_w A_{w\lambda}]^c}, \quad (4.9)$$

in which the product $m_w w$ represents the slant water vapour column, where m_w adjusts for the increased path length when the sun is not at zenith and w (cm) is the precipitable water

vapour². The exponent 1.05 applied to this term is an empirical correction which accounts for the non linearity in absorption efficiency, as the amount of water vapour increases. The factor $(f_w)^n$ introduces a correction for pressure or temperature broadening, where f_w is a wavelength-dependent scaling factor related to atmospheric conditions and n is an empirical exponent. B_w is an empirical fitting constant that depends on the air mass and is used to adjust the amplitude of the absorption. The spectral dependence of absorption is introduced by $A_{w\lambda}$, which accounts for the strong variation of water vapour with wavelength. Finally, the exponent c is another empirical parameter used to adjust the shape or curvature of the resulting transmittance curve, allowing the expression to closely match detailed radiative transfer results without the associated computational cost of a radiative transfer model. Further description of these parameters can be found in Appendix B.11.

Aerosol transmittance

The effects of absorption and scattering (i.e. attenuation) by aerosols are modelled following the approach of (Bird and Riordan, 1984), which divides the solar spectrum in two regions: 1-below and 2-above a critical wavelength, $\lambda_0 = 500$ nm. This separation reflects the fact that aerosol interactions with radiation depend on particle size and wavelength (see Section 2.2). The choice of λ_0 , near the maximum of the solar spectra, marks the transition from Rayleigh to Mie scattering. This method, known as the modified Ångström approach, simplifies aerosol modelling by treating small and large particles separately. The aerosol transmittance, $T_{a\lambda}$, is calculated as:

$$T_{a\lambda} = e^{-m_a \tau_{a\lambda}}, \quad (4.10)$$

where the aerosol optical depth ($\tau_{a\lambda}$) is modelled using the Ångström Law (Eq. 2.23) applied in two spectral ranges ($i = 1, 2$):

$$\tau_{a\lambda} = \beta_i \left(\frac{\lambda}{\lambda_1} \right)^{-\alpha_i} = \begin{cases} 2^{\alpha_2 - \alpha_1} \left(\frac{\lambda}{\lambda_1} \right)^{-\alpha_1} & \text{for } \lambda < \lambda_0, \\ \beta \left(\frac{\lambda}{\lambda_1} \right)^{-\alpha_2} & \text{for } \lambda \geq \lambda_0. \end{cases} \quad (4.11)$$

In Eq. (4.11), λ/λ_1 is a dimensionless factor, λ_1 is the reference wavelength, λ is the variable wavelength and λ_0 is the transition wavelength. If λ_1 is expressed in nm, then coherently, λ must be expressed in nm.

To be able to solve Eq. (4.11), specific parameters for each band α_1 , α_2 , and β must be determined previously. For this purpose, two different user inputs are required: the aerosol model, which relates to the computation of α_1 , α_2 , and the turbidity which is related to the computation of β .

²Notice the precipitable water vapour is expressed in cm because it represents the depth of liquid water that would result if all the water vapour in a vertical column of the atmosphere was condensed. This depth is calculated under standard temperature and pressure conditions (STP, temperature of 0° or 273.15 K and 1 atm or 101325 Pa), providing a physically intuitive and consistent measure.

Regarding α_i , Fig. 4.4 shows the behaviour of $\tau_{a\lambda}$ vs. λ , when Eq. (4.11) is applied in two cases: modelling $\tau_{a\lambda}$ in two spectral regions or in a single spectral region. For the first case, typical values are used: $\alpha_1 = 1.3$, $\alpha_2 = 0.8$ and $\beta = 0.2$. It is observed that $\tau_{a\lambda}$ decreases as the wavelength increases, following an Ångström power law. The change in slope that occurs at the transition wavelength, $\lambda_0 = 675$ nm, reflects the shift from fine-mode to coarse-mode aerosols. When instead, $\tau_{a\lambda}$ is modelled with only one α , for example with values: $\alpha = 1.3$, and $\beta = 0.2$, the model becomes a continuous curve. It is computed that for a reference wavelength of $\lambda_0 = 500$ nm, at $\lambda = 500$ nm, $\tau_{a\lambda}$ acquires a value of 0.2 in the case of a one step curve, and 0.14 in the case of a two-steps curve.

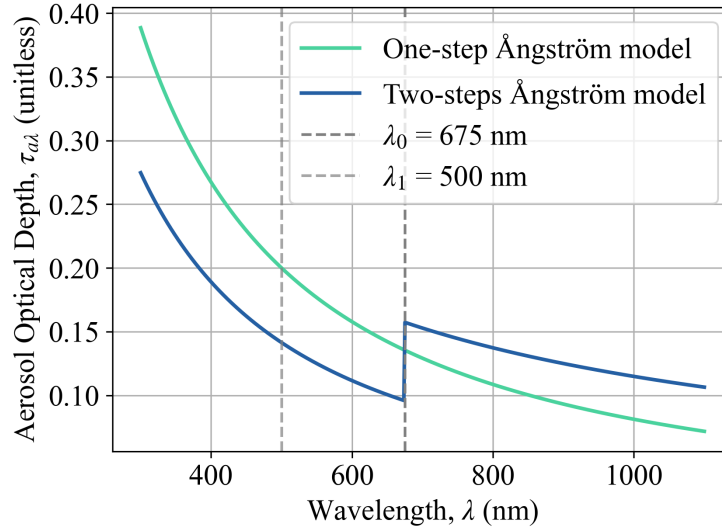


Figure 4.4: Two possible Ångström parametrizations used in SMARTS (Gueymard, 1995). Green: generated using Ångström coefficients $\alpha_2 = 1.3$, $\beta = 0.2$. Blue: generated using $\alpha_1 = 1.3$ (for $\lambda < \lambda_0$, fine particles), $\alpha_2 = 0.8$ (for $\lambda \geq \lambda_0$, coarse particles), $\beta = 0.2$, $\lambda_0 = 675$ nm, $\lambda_1 = 500$ nm. Figure by Paola Russo.

If specific values for α_i are not available, SMARTS provides several aerosol models that define the wavelength dependence of $\tau_{a\lambda}$. Each model uses its own empirical values of α_1 and α_2 , allowing SMARTS to represent different aerosol conditions. Among these aerosol models, there are Shettle and Fenn (1979) (S&F, with variations: rural, urban, maritime and tropospheric) and (Braslau and Dave, 1973) (B&D). These options have pre-loaded values for α_1 and α_2 , depending on the relative humidity. Particularly, S&F tabulated values are shown in Table B.6 since this is the model used in this work, because it is the one that offers a better performance in this region. Additionally, the aerosol model parameters can also be specified manually as user input, providing the parameters: α_1 , α_2 , Single Scattering Albedo (w_0) and Aerosol Asymmetry

parameter (g) (for definitions of w_0 and g , see Appendix B.6, and for typical values for w_0 , see Appendix B.7, Table B.2).

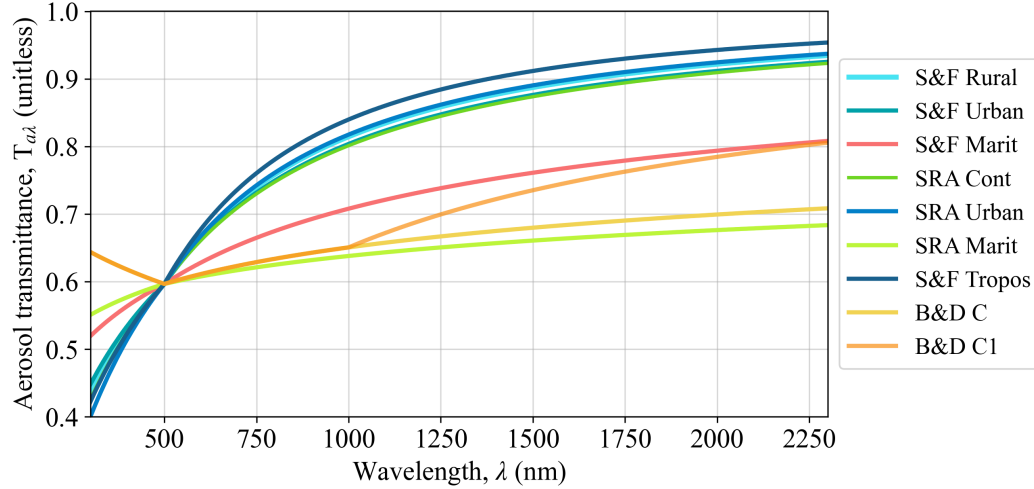


Figure 4.5: Aerosol transmittance models from (Braslau and Dave, 1973; IAMAP, 1986; Shettle and Fenn, 1979). Modelled with SMARTS (Gueymard, 1995) using STS reference atmosphere, $m = 1.5$, $\tau_{a500} = 0.3442$. Figure by Paola Russo.

Figure 4.5 shows the different aerosol transmittance curves generated with SMARTS for the different aerosol models, depending on the wavelength. S&F models display smooth attenuation, with the Rural and Tropospheric variants exhibiting higher transmittance due to lower aerosol loading, while the Urban and Maritime models show slightly stronger attenuation, especially in the UV-visible range, reflecting higher particle concentrations or humidity growth effects. The SRA models also differ, with the Urban and Maritime types generally presenting lower transmittance than the Continental, which assumes cleaner, drier air masses. The BD models, particularly C1, reveal more abrupt spectral features and an unusual dip in the visible, which is likely due to empirical parametrization and not necessarily physical aerosol behaviour. In contrast, the user-defined aerosol model, yields a flexible and interpretable transmittance shape, allowing tailored representation of specific atmospheric conditions. These differences highlight how each model implicitly assumes different aerosol size distributions, chemical compositions, and concentration levels, and they should be chosen according to the atmospheric context under study.

Regarding the turbidity, it can be directly loaded as an input parameter through β (or aerosol optical depth at 1000 nm) or it can be given through other input parameters that the model converts into β , using Eq. (4.12). The other options are: aerosol optical depth at 500 or 550

nm (τ_{a500} , τ_{a550}), Schüep's turbidity coefficient (B , or decadic aerosol optical depth at 500 nm), meteorological range (VR) based on Koschmieder's equation (Koschmieder, 1924), or the prevailing visibility (V) observed at airports. In this work, the option selected is using τ_{a550} as a variable input and letting the model calculate β .

$$\begin{aligned}
 B &= \tau_{a500} / \ln 10 \\
 \beta &= (0.5^{\alpha_2}) \\
 \tau_{a500} &= (0.55^{\alpha_2}) \tau_{a550} \\
 \text{VR} &= 1.306 V \\
 \beta &= (0.55^{\alpha_2}) f(\text{VR})
 \end{aligned} \tag{4.12}$$

4.1.2. Diffuse spectral irradiance

Diffuse radiation $G_{dh,\lambda}$ in the SMARTS model is considered as the sum of parts originated in three processes: Rayleigh scattering ($G_{dhR,\lambda}$), aerosol scattering ($G_{dha,\lambda}$), and ground/background scattering ($G_{dhs,\lambda}$),

$$G_{dh,\lambda} = G_{dhR,\lambda} + G_{dha,\lambda} + G_{dhs,\lambda}. \tag{4.13}$$

In what follows, each component part is described.

Rayleigh scattering component

The diffuse spectral irradiance due to Rayleigh scattering, $G_{dhR,\lambda}$, is derived from the direct extraterrestrial spectral irradiance, $G_{0h,\lambda}$, attenuated by molecular scattering losses, as expressed in

$$G_{dhR,\lambda} = F_R G_{0h,\lambda} \left[1 - (T_{r\lambda})^{0.9} \right] \Gamma_{o\lambda} T_{n\lambda} T_{g\lambda} T_{w\lambda} T_{aa\lambda} \cos \theta_z. \tag{4.14}$$

The term $\left[1 - (T_{r\lambda})^{0.9} \right]$ quantifies the fraction of radiation scattered by air molecules. This expression is further modulated by several atmospheric transmittances, including those of ozone ($\Gamma_{o\lambda}$), nitrogen, water vapour, and aerosols (Table 4.1). The $\cos \theta_z$ factor accounts for the transposition to horizontal plane, while the angular redistribution of Rayleigh-scattered irradiance is represented by the correction factor F_R , which adjusts for the fraction of scattered irradiance that reaches the surface.

The effective ozone transmittance, $\Gamma_{o\lambda}$, in Eq. (4.14), represents an approximation to the transmittance of ozone, and is calculated differently from $T_{o\lambda}$ or the rest of transmittances. Empirical evidence (Gueymard, 2001) suggests that the depletion of downward diffuse radiation due to ozone does not follow the Lambert's Law, which applies to beam solar irradiance on a well defined path. The difference is identifiable particularly in the UV-B region, where absorption of diffuse irradiance is stronger and non linear, and at large zenith angles, where the path length through

the atmosphere increases, and scattering dominates. In those cases, applying an exponential decay as Lambert's Law would underestimate the diffuse attenuation by ozone, instead, $\Gamma_{o\lambda}$ allows for a better fit to the observations. SMARTS calculates $\Gamma_{o\lambda}$ using a parametrization dependant on the ozone relative air mass, m_o , described in Appendix B.5, and (Gueymard, 1995).

Another empirical factor that appears in Eq. (4.14) is 0.9. It has been observed that in a real atmosphere, there is an excess of lateral dispersion, that is not captured by simply $[1 - (T_{r\lambda})]$, therefore, an empirical adjustment factor, exponent 0.9, is applied to $T_{r\lambda}$ (Gueymard, 2001). In

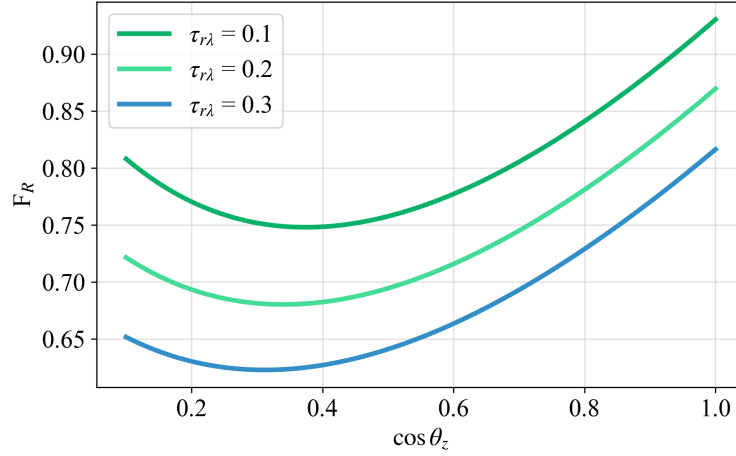


Figure 4.6: Downward angular correction factor for Rayleigh-scattered irradiance, F_R , for different $\tau_{r\lambda}$ values, and different $\cos \theta_z$ angles. Figure by Paola Russo.

real conditions, how much Rayleigh-scattered irradiance actually reaches the ground, depends on how much scattering occurs ($\tau_{r\lambda}$) and from what direction the beam irradiance is coming (θ_z). Because of this, an angular correction factor, the downward fraction of Rayleigh-scattered radiation (F_R) that depends on $\tau_{r\lambda}$ and θ_z is applied (see Appendix B.4 for details). $F_R = F_{R1} \times F_{R2}$ where $F_{R1} = 0.5$ represents the fraction of radiation scattered downward under the assumption of isotropic single scattering, and F_{R2} applies a correction to account for multiple scattering based on $\tau_{r\lambda}$ and θ_z , F_R . Therefore, SMARTS models as if approximately half of the scattered energy (related to F_{R1}) is redirected downward toward the ground, while the rest escapes to space. The F_{R2} term adjusts this proportion to account for enhancement or reduction due to multiple scattering events. To analyse this, Fig. 4.6 shows the behaviour of F_R versus $\cos \theta_z$ for different values of $\tau_{r\lambda}$. It is observed that F_R (excluding low sun conditions with $\cos \theta_z < 0.3$) increases as the sun rises ($\cos \theta_z \rightarrow 1$) allowing a greater fraction of Rayleigh-scattered irradiance to reach the surface. Another observation is that for a fixed θ_z (for example, $\cos \theta_z = 0.4$), F_R decreases as $\tau_{r\lambda}$ increases. This is expected because of low Rayleigh optical depth (for example $\tau_{r\lambda} = 0.1$), Rayleigh scattering is weak, in that case single scattering becomes

dominant and F_{R1} dominates the F_R equation, providing a greater value of F_R , that means the fraction of photons scattered in the direction of the ground (downward scattered) is greater (as observed in the green curve, with values of F_R near 0.75). On the other hand, for high $\tau_{r\lambda}$ (for example $\tau_{r\lambda} = 0.3$), photons undergo more scattering events, some photons that were initially scattered downward are re-scattered sideways or upward, obtaining a net effect of more photons eventually escaping in directions other than downward and F_{R2} decreases the final value of F_R accordingly. As a result, the fraction of scattered photons reaching the ground decreases slightly (as observed in the blue curve, with values near 0.63).

The aerosol absorption transmittance, $T_{aa\lambda}$, is a factor that quantifies how much irradiance still passes through the atmosphere, once aerosols have absorbed a part of it, it is calculated as:

$$T_{aa\lambda} = e^{-m_a(\tau_{a\lambda} - \tau_{as\lambda})} \quad (4.15)$$

where m_a is the aerosol optical air mass, $\tau_{a\lambda}$ is the total aerosol optical depth, and $\tau_{as\lambda} = w_0 \times \tau_{a\lambda}$ represents how much is scattered. The difference $\tau_{a\lambda} - \tau_{as\lambda}$ is an effective optical thickness that corresponds to the amount of irradiance absorbed by aerosols.

Aerosol scattering component

Aerosol scattering is modelled as a fraction of the reference beam normal irradiance, $G_{0h,\lambda}$, that is transmitted downwards.

$$G_{dha,\lambda} = F_a G_{0h,\lambda} (1 - T_{as\lambda}) \Gamma_{o\lambda} T_{r\lambda} T_{n\lambda} T_{g\lambda} T_{w\lambda} T_{aa\lambda} \cos \theta_z \quad (4.16)$$

where: F_a is the fraction of the scattered flux that is transmitted towards the ground direction, its computation is shown in (Gueymard, 1995). $T_{as\lambda} = \frac{T_{a\lambda}}{T_{aa\lambda}}$ is the transmittance of aerosol scattering, $T_{aa\lambda}$ is the transmittance of aerosol absorption and $T_{a\lambda}$ is the total transmittance due to aerosol attenuation.

Conceptually, Eq. (4.16) models how solar radiation that has been scattered by aerosols in the atmosphere, reaches the ground surface in the form of diffuse irradiance. For this, it considers that only a fraction of the beam solar radiation that enters the atmosphere $G_{0h,\lambda}$ is scattered towards the downward direction (thus the multiplication by F_a). Additionally, from that portion only a part $(1 - T_{as\lambda})$ is scattered by aerosols before reaching the ground surface ($T_{as\lambda}$ represents the fraction of radiation that is transmitted without being scattered by aerosols). Later, this scattered part, also suffers the effects of atmospheric scattering and absorption due to ozone, aerosols, gases, and Rayleigh scattering ($\prod_i T_i$), until it reaches the ground surface. The factor $\cos \theta_z$ is for calculating the horizontal projection.

Backscattering component

The diffuse backscattering component of the spectral irradiance, $G_{dhs,\lambda}$, accounts for the radiation that has been reflected multiple times between the ground and the atmosphere before

reaching the observer. It is expressed as

$$G_{dhs,\lambda} = \frac{\rho_{s\lambda} (\rho_{b\lambda} G_{b,\lambda} \cos \theta_z + \rho_{d\lambda} G_{dh0,\lambda})}{(1 - \rho_{d\lambda} \rho_{s\lambda})}. \quad (4.17)$$

The first component of $G_{dhs,\lambda}$ is the isotropical reflection of horizontal beam irradiance by the ground, $\rho_{b\lambda} G_{b,\lambda} \cos \theta_z$, where $\rho_{b\lambda}$ is the spectral reflectance for beam irradiance (in a characteristic area of less than 100 km²). To this, the amount of reflected diffuse radiation by the ground that is scattered back into the atmosphere is added. This term is calculated by decreasing the reference diffuse irradiance $G_{dh0,\lambda}$ (the amount of diffuse solar radiation reaching the surface, assuming an ideally non-reflective surface) by the spectral reflectance for diffuse radiation, $\rho_{d\lambda}$. Since both components go through an infinite series of reflections between the ground and the atmosphere, the factor $\rho_{s\lambda}/(1 - \rho_{d\lambda} \rho_{s\lambda})$ appears as the summation of a geometric series, where the sky overall spectral reflectance is $\rho_{s\lambda}$. More details on this can be found in Appendix B.8.

4.1.3. SMARTS outputs

SMARTS can generate different sorts of outputs depending on the user needs. The raw output is the spectral irradiance ($G_{h,\lambda}$, $G_{dh,\lambda}$, $G_{b,\lambda}$, W/m²μm) estimated in the 280-4000 nm range. It has a variable spectral resolution that ranges from 1 nm (in the smaller wavelengths up until 1700 nm) to 5 nm (in the infrared up until 4000 nm). Integrating the raw output in the wavelength range 280-4000 nm leads to broadband irradiance (G_h , G_{dh} , G_b , W/m²), which is comparable with a broadband instrument's measurement such as a pyranometer or pyrheliometer. Other band-specific outputs can also be obtained from integration in the corresponding wavelength regions, for example all the components of PAR are obtained integrating the raw output in the 400-700 nm wavelength range, the UV in the 280-400 nm and NIR in 700-1000 nm. In order to calculate $G_{h,\lambda}$, SMARTS uses the estimates for $G_{dh,\lambda}$ and $G_{b,\lambda}$ and applies the closure relation from Eq. 2.6 (explained in Section 2.1):

$$G_{h,\lambda} = G_{b,\lambda} \cos \theta_z + G_{dh,\lambda}. \quad (4.18)$$

Then, G_h , G_{dh} and G_b are computed from the integral of these estimates.

SMARTS also allows the user to model the response a real collimated spectroradiometer would have if it measured at ground level. For this, it generates a smoothed beam spectral irradiance output (W/m²μm), and also estimates circumsolar radiation. The smoothing method performs a Gaussian convolution of the raw output, centred in the wavelength of interest and with width FWHM (Full Width at Half Maximum), which is a customizable parameter. Further information on the convolution method and what the FWHM represents is available in Appendix B.13. Along with this procedure it is possible to estimate the circumsolar irradiance that the spectroradiometer would measure, and also correct the smoothed irradiance estimation in order to account for it. For this, it is required to enter the specific geometry parameters of the collimator tube, such as slope angle, aperture angle or limit angle (see Appendix A.1 for a scheme of where

these parameters are located). It is important to notice that the smoothed output is the only output comparable to a spectroradiometer's measurement, as explained in the documentation (Gueymard, 2005).

4.1.4. Previous assessments

The performance of SMARTS has been evaluated in the literature for several locations worldwide. The papers discussed here have been selected for presenting quantitative results of bias and dispersion in broadband terms, Eq. (2.26) and in spectral terms, Eq. (2.28). Some of them show results of global, diffuse and beam irradiance, as well as different atmospheric data sources.

It is important to notice that comparing assessments from different studies is not straightforward due to varying metrics and methodologies. Different kinds of comparisons are found in the literature: (i) using to broad-band irradiance measurements or estimates, (ii) with solar spectral irradiance from surface measurements or (iii) reporting consistency with other spectral irradiance models as reference, usually detailed radiative transfer models.

Regarding broadband performance, Table 4.2 shows performance results of SMARTS obtained by previous authors, for the variables G_h , G_{dh} and G_b , using different atmospheric data sources: AERONET (AERO), MERRA-2 (ME-2) and Copernicus Atmospheric Service (CAMS). In general, there is plenty of literature for G_h and G_b but there are few reported results for G_{dh} . In that sense, the only work that was found is from (Askar and Batty, 2005), where the G_{dh} is modeled with SMARTS and then compared to ground measurements in Kuwait. However, unfortunately its results are presented as a plot, so the MBD and RMSD shown in Table 4.2 have been obtained from digitalizing the plot and calculating a numeric value, with the due uncertainty this estimation may introduce. From analyzing Table 4.2, the first conclusion is that the atmospheric inputs play an important role in the performance of SMARTS. For the variable G_b , using AERO outperformed using ME-2 or CAMS almost in every case, improving bias and also dispersion, this is explainable because AERO consists of retrievals from ground measurements, whereas ME-2 and CAMS are reanalysis data bases, which can have more sources of uncertainty. Additionally, their time intervals vary, being another possible source of uncertainty. Comparing G_h to G_b shows that both variables share similar biases and dispersions magnitudes, however it is noticed that G_b often has a negative bias, regardless of its atmospheric data source, and G_h always has a positive bias. Perhaps biases of G_{dh} and G_b are being compensated, but this can only be an hypothesis, since (Salmon et al., 2021) and Ruiz-Arias et al. (2019) do not show results for G_{dh} . On the other hand, the only result for G_{dh} draws the attention towards it and also its large dispersion, however this values may be related to either ground measurements large uncertainties or uncertainties in the calculus of performance from the image. Still, qualitatively speaking, it can be said that the bias is negative.

Regarding spectral performance, SMARTS outputs have been compared to ground measurements in previous studies, however, few works show exhaustive quantitative results on the per-

Table 4.2: Broadband performance of SMARTS G_h , G_{dh} and G_b estimates expressed as a % of the average measured G_h . The metrics are defined in Eq. (2.26). The data sources are abbreviated as: Sa21: Salmon et al. (2021), RA19: Ruiz-Arias et al. (2019), Ab23: Abreu et al. (2023), As5: Askar and Batty (2005). Atmospheric data sources are abbreviated as: AERONET (AERO), MERRA-2 (ME-2), Copernicus Atmospheric Service (CAMS). Climatic classifications according to Köpen Geiger (Prša et al., 2016).

Site	Climate	Atmos. input	rMBD (%)	rRMSD (%)	$< G_h >$ (W/m ²)	Source
G_h						
Évora, Portugal	Csa	AERO	2.5	3.0	483.9	Ab23
		ME-2	1.1	2.3		
		CAMS	2.2	3.0		
G_{dh}						
Kuwait	BWh	Meas.	-14.7	31.3	186.4	As5
G_b						
Cabaw, Netherlands	Cfb	AERO	2.3	4.9	633.0	Sa21
Carpentras, France	Cfb		-0.2	1.6	732.5	
Palaiseau, France	Cfb		-0.4	2.3	693.7	
Sao Martinho, Brazil	Cfa		-3.5	5.4	784.1	
Solar Village, Saudi Arabia	BWh	AERO	-7.1	7.7	662.4	RA19
		ME-2	-9.8	13.1		
Tamanrasset, Algeria	BWh	AERO	-1.3	3.2	696.5	
		ME-2	-9.8	17.3		
Sede Boker, Israel	BSh	AERO	-4.6	5.6	738.0	
		ME-2	-7.3	9.7		
Gobabeb, Namibia	BSh	AERO	-0.2	1.5	850.7	
		ME-2	-5.7	8.7		
Évora, Portugal	Csa	AERO	1.2	1.9	798.7	Ab23
		ME-2	-2.3	4.6		
		CAMS	3.1	5.4		

formance of $G_{h,\lambda}$, $G_{dh,\lambda}$ and $G_{b,\lambda}$. This could be because ground surface spectral irradiance measurements of high quality are scarce. Among these studies, Apell and McNeill (2019) evaluated the performance of $G_{b,\lambda}$ estimates from SMARTS by comparing them with ground measurements. The study was conducted in four sites: Golden (NREL³, Colorado, USA), Boulder (NOAA⁴, Colorado, USA), Barrow (NSF, Alaska, USA) and Ushuaia (NSF⁵, Argentina). Mea-

³National Renewable Energy Laboratory (NREL).

⁴National Oceanic and Atmospheric Administration (NOAA).

⁵National Science Foundation (NSF).

measurements were taken during four days, distributed in all seasons (March 23, June 19, September 24, December 19), for Golden and Boulder, and during summer for the poles. No smoothing was applied to the model outputs, instead, raw outputs were evaluated. Each site spectroradiometers had different spectral ranges, as shown in Table 4.3. It was concluded that the model had a good agreement with measurements in all sites, observing only small discrepancies in the spectra. Spectral performance metrics were not presented. In Golden, discrepancies were found in the O₂ band (760 nm) and the *w* band ($\sim 715 - 735$ nm). In Boulder, the model overestimated measurements, what is explained by an underestimation in ozone. In both pole sites, the spectral concordance was very good, and there was only an underestimation in the region of 310 nm, explained by an overestimation of ozone.

Table 4.3: Summary of SMARTS spectral comparisons from Apell and McNeill (2019).

Site	Range (nm)	Time	Results
Golden, Co., USA	300–800	4 days, daily averages	Good agreement
Boulder, Co., USA	280–450	Solar noon; 4 days	< 310, 760, 715-735 nm
Barrow, Ak., USA	280–600	Summer	Good agreement
Ushuaia, Argentina	280–600	Summer	Good agreement

In another study, Utrillas et al. (1998) evaluated the performance of SMARTS estimates of $G_{b,\lambda}$ against ground measurements at a site in Valencia, Spain. Measurements were taken using a LiCor 1800 spectroradiometer, within the wavelength range of 300–1100 nm. The data set consisted of 60 instants from ten clear-sky days, spanning from January to March. The model was executed for nine aerosol model options, including S&F Rural and Urban. Results indicate that the optimal $G_{b,\lambda}$ estimates were obtained with S&F Urban, S&F Rural, SRA-C⁶ and SRA-U. The mean MBD (%) and RMSD (%) obtained are shown in Table 4.4.

Table 4.4: Performance metrics of SMARTS estimates in Valencia, Spain (Utrillas et al., 1998).

	MBD (%)	RMSD (%)
S&F Rural	0.9	6.0
S&F Urban	-0.0	6.7
SRA-C	0.4	6.0
SRA-U	0.8	5.4

Kaskaoutis and Kambezidis (2008) highlights the importance of the aerosol model on the accuracy of SMARTS. To understand its impact, spectral measurements (320 - 1000 nm) made during May 1995 in Athens, Greece (a coastal site in the Mediterranean), were used to test

⁶Standard Radiation Atmosphere, Continental (SRA-C) and Urban (SRA-U).

Table 4.5: Performance of G_b from SMARTS v2.9.2 discriminated by spectral bands, when using different aerosol models in Athens, Greece (Kaskaoutis and Kambezidis, 2008). Spectral performance indicators are based on the relative residuals, as defined in Eq. (2.31). rMBD and rRMSD are expressed in percentage (%) relative to the mean observed values.

band	range (nm)	SF-Urban		SF-Rural		SF-Maritime	
		rMBD	rRMSD	rMBD	rRMSD	rMBD	rRMSD
UV	320-400	19.4	26.3	10.1	20.8	50.1	53.8
VIS	400-700	-3.9	9.6	-6.9	11.2	5.9	11.9
NIR	700-1000	-4.4	16.1	-4.8	16.1	-3.1	16.0
Total	320-1000	-2.0	14.8	-4.6	14.5	6.7	21.2

SMARTS v2.9.2 estimates of $G_{b,\lambda}$. The analysis was based on the best 26 spectra from a much larger data set, in order to minimize uncertainties. Mostly default values, based on the chosen atmospheric model, were used as atmospheric inputs except for AOD_{500} which was retrieved from the measured spectral irradiance using methods similar to those described in 6. The focus of this analysis was to compare performance in three sub-bands (UV, VIS and NIR) for three frequently used SF aerosol models (Urban, Rural, Maritime). The results are summarized in Table 4.5. Large positive biases (overestimation) were found in the UV band for all aerosol models, especially for the SF-Maritime model. Smaller negative biases (underestimation) were found in the other bands, with the exception of the VIS band with the Maritime model. A similar earlier study (Utrillas et al., 2000) used 500 $G_{b,\lambda}$ spectra for Valencia, Spain and several aerosol models with similar results (although with lower performance indicators). These results highlight the importance of selecting an adequate aerosol model for each site.

In another assessment, Myers and Gueymard (2004) evaluated the performance of SMARTS using spectral irradiance measurements from the Solar Spectral Database (SSDB) and from NREL calibration campaigns in Colorado. The data set consisted in 644 spectra: 144 measured at FSEC (Florida), San Ramon (California), and Denver (Colorado) during 1987-1988, using LiCor Li-1800 spectroradiometers, and 500 additional clear-sky spectra collected at NREL. The Li-1800 instrument had a spectral range of 400-1100 nm, with a nominal resolution of 6 nm. The comparison showed that SMARTS estimates were generally within the instrumental uncertainty ($\sim 5\%$) across most of the Li-1800 range, indicating good spectral agreement between modelled and measured irradiance. However, the study does not report MBD or RMSD values for each site.

In Gueymard (2008a) SMARTS is compared to models such as MODTRAN or LibRadTran, which solve the radiative transfer equation rigorously. For this, all the models are executed with the same atmospheric input conditions (aerosol properties, ozone, water vapour). Then, the $G_{b,\lambda}$ estimates produced by each model are compared to SMARTS, showing their percentage differences. As results, spectral differences remain below $\pm 1\text{-}2\%$ across almost all the spectrum,

except for the strong absorption bands of water vapour and O_2 . This is coherent with what is reported in the official website from SMARTS, where it is stated that the model was developed to coincide with the MODTRAN model in relevant bands, within 2 %. Other works such as Gueymard (2001) and (Gueymard, 2005) also compare SMARTS outputs with RTE models, but not so rigorously.

From the previous assessments presented, it is observed that there are few performance analysis of SMARTS in the region of South America. Furthermore, it is also identified that there are few comparisons to ground measurements of $G_{h,\lambda}$, $G_{dh,\lambda}$, and $G_{b,\lambda}$. The lack of research in those areas motivate their study in the following section.

4.2. Methodology

A scheme of the workflow is presented in Fig. 4.7. The methodology to perform the assessment of SMARTS consists of successive steps: 1) preparing atmospheric inputs from different data sources, 2) applying the SMARTS model and obtaining different outputs, 3) comparing to ground quality controlled measurements, for a performance analysis. The spectral study and the broadband study will consider different datasets, since the amount of available measurements as well as the procedures proposed are different. A thorough description of the procedures proposed will be provided for each case. Furthermore, in what follows, all the steps outlined in Fig. 4.7 will be described in detail.

4.2.1. Broadband and spectral irradiance ground measurements

Spectral comparisons

Spectral measurements are used to compare the model spectral estimates: $\hat{G}_{h,\lambda}$, $\hat{G}_{dh,\lambda}$ and $\hat{G}_{b,\lambda}$ to corresponding ground measurements of $G_{h,\lambda}$, $G_{dh,\lambda}$ and $G_{b,\lambda}$. A new EKO MS711 spectroradiometer is used as the main instrument to measure $G_{h,\lambda}$, $G_{dh,\lambda}$ (using a variation of the "shade and unshade method") and $G_{b,\lambda}$ is estimated from the closure relation. Measurements of $G_{h,\lambda}$ and $G_{dh,\lambda}$ are taken near solar noon, following a one-minute alternating shading/unshading cycle of the instrument's dome as explained below.

The EKO MS711N instrument is mounted on a SOLYS2 sun tracker equipped with a shadow ball, located at LES (see Section 2.4 and Table 2.2 for details). The experiment is performed during 18th June 2024, between 11:15 and 13:41, corresponding to the day of year: $n = 170$ during winter season, with cosines of the zenith angle (θ) ranging from 0.509 to 0.562 and air masses between 1.96 and 1.77.

The measurement scheme is shown in Fig. 4.9. First, $G_{dh,\lambda}$ is measured with the instrument's sensor shaded under the shadow ball during minute i , as shown in Fig. 4.8 (b). On the next minute ($i + 1$), the shadow ball is manually removed and $G_{h,\lambda}$ is measured in unshaded conditions, as

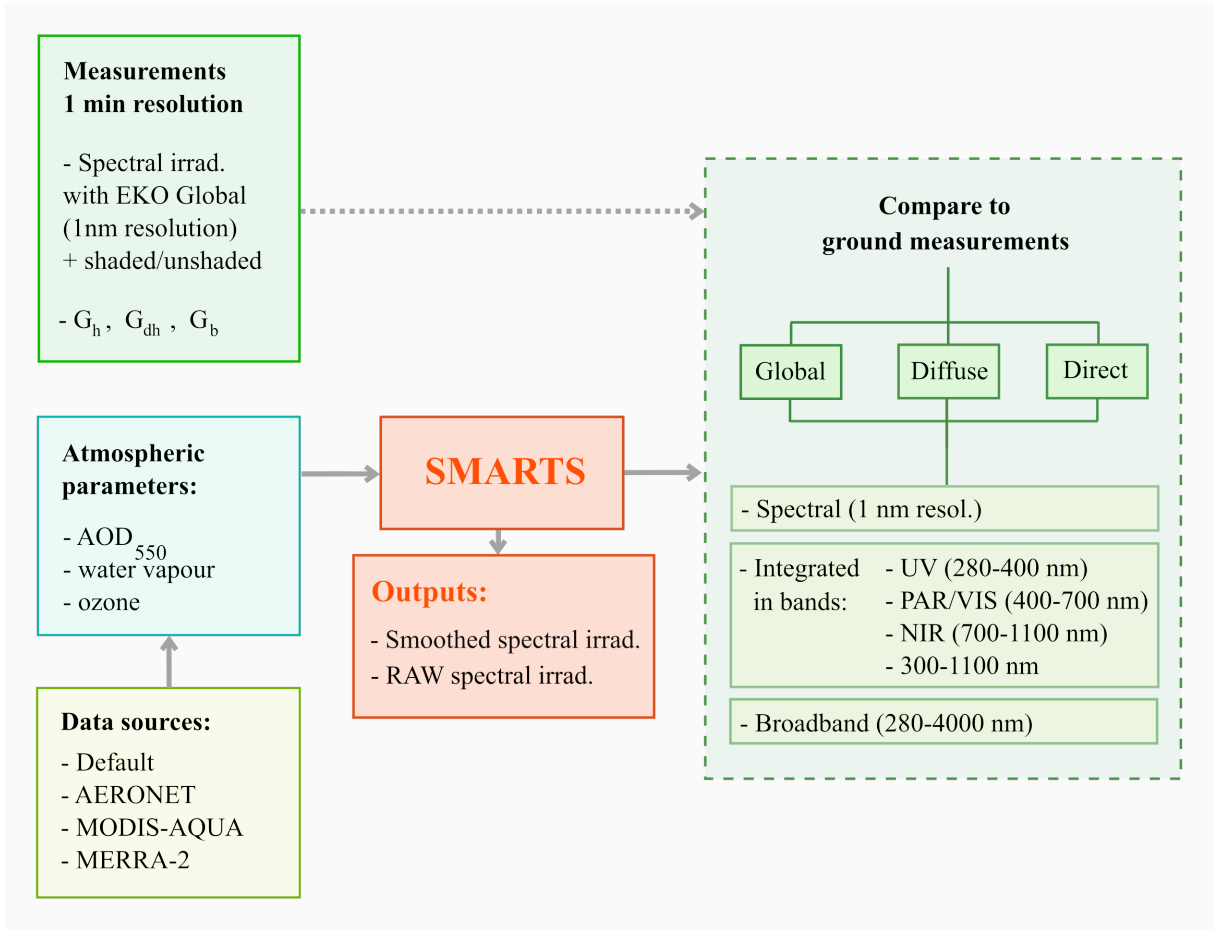


Figure 4.7: Workflow diagram for SMARTS assessment. Figure by Paola Russo.

shown in Fig. 4.8 (a). The procedure is repeated during several consecutive instants around the solar noon on a clear-sky day. The remaining component, $G_{b,\lambda}$, is calculated applying closure (Eq. 2.6) during the shaded instant (i):

$$G_{b,\lambda}(i) = \frac{G_{h,\lambda}(i+1) - G_{d,\lambda}(i)}{\cos \theta_z(i)} \quad (4.19)$$

In this scheme it is assumed that $G_{h,\lambda}(i) \simeq G_{h,\lambda}(i+1)$. The error of this assumption is minimal, if measurements are taken near solar noon on a clear sky day, because the atmospheric conditions remain almost invariable at 1 minute intervals, and the air mass varies little.

Measurements are taken processed and quality checked, based on visual inspection of the spectral data and the integrated spectral data (in the range 300-1100 nm), combined with the shaded/unshaded classification from the metadata, with the objective of discarding any erroneous

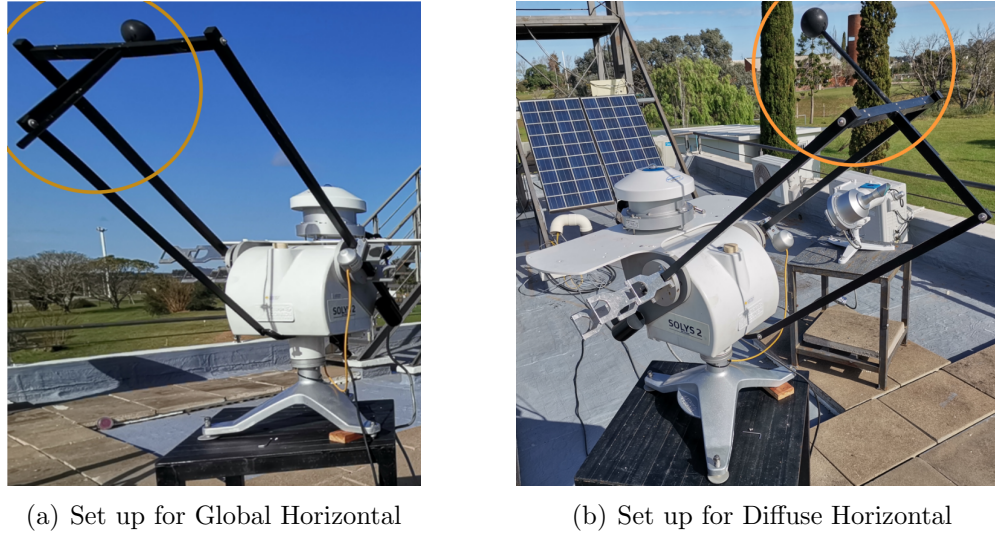


Figure 4.8: Spectroradiometer EKO MS-711N used for measuring Global Horizontal and Diffuse Horizontal spectral irradiance at ground level (without and with shadow ball mounted respectively). Figure by Paola Russo.

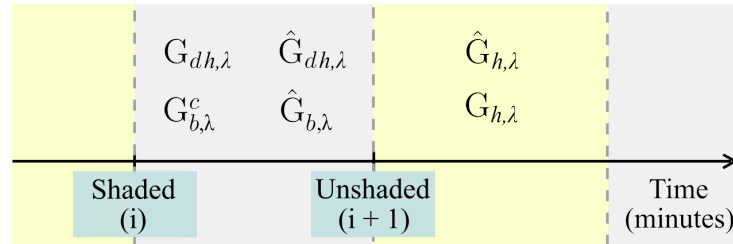


Figure 4.9: Shaded-unshaded scheme used for the performance comparisons. The scheme shows the modelled (hat) and observed variables representative of the whole interval but they are actually assigned to the start of their interval, as it is a conventional practice. Spectral dependence is implied in all the variables. The superscript c indicates that variable is obtained using closure (Eq. 2.6). Figure by Paola Russo.

measurements (for example: mistakenly annotated as shaded when it was unshaded). After these checks are applied all instants are assured to be of clear sky and stable atmospheric conditions. Figure 4.10 shows the 112 instants selected, from which 56 correspond to unshaded conditions and 56 to shaded conditions. Measurements are afterwards used in the performance analysis. The performance of the spectral model is quantified in terms of spectral MBD and RMSD (Eq. 2.28).

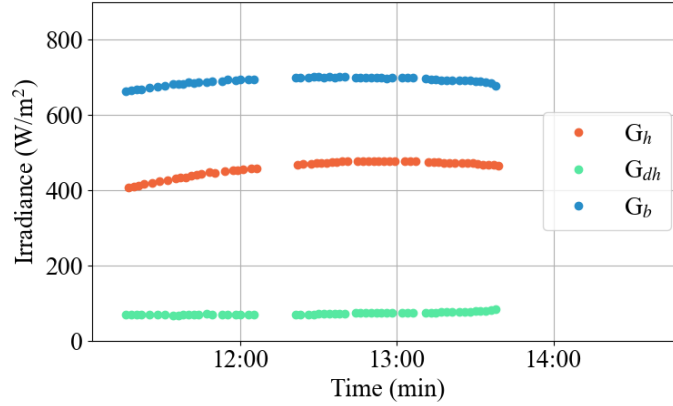


Figure 4.10: Time series of the three components of the spectral irradiance integrated in 300-1100 nm: global horizontal (G_h), diffuse horizontal (G_{dh}) and beam normal (G_b), during day 2024/06/18. Figure by Paola Russo.

Broadband comparisons

Broadband performance is calculated comparing the SMARTS broadband model against broadband irradiance ground measurements. SMARTS broadband variables⁷ are obtained by aggregating $\hat{G}_h$, $\hat{G}_{dh}$ and $\hat{G}_b$ over the 280-4000 nm spectral range, as defined in Eq. (2.3). The performance is quantified in terms of rMBD and rRMSD, Eq. (2.26). For this, 1 minute broadband measurements of G_h , G_{dh} and G_b are used from the LES routine measurements (see Section 2.4).

The performance analysis is done comparing the model outputs of G_h , G_{dh} and G_b ground measurements. The samples come originally from a 1 minute sampling frequency data set of 2,630,880 individual samples of each variable, from 2020-01-01T00:00 to 2024-12-31T23:59. From this data set, a subset of 28 days with clear-sky and stable atmospheric conditions is selected, using visual inspection. The inspection includes observing G_h , G_{dh} and G_b simultaneously with the atmospheric parameters AOD, w and u_o , to identify the desired periods where clear-sky and stable atmospheric conditions are met. Once this clear-sky selection is done, the number of samples is decreased, so that it is possible to model a manageable amount of instants. For this, one sample every 4 minutes is selected (the values are kept instantaneous, not averages). This leads to a final selection of 2296 individual samples, equally distributed during 5 years, during all seasons, and covering zenith angles from sunrise to sunset. Additional information on this selection of instants is described in Appendix C.3 along with basic descriptive statistics (such as minimum, maximum, average and standard deviation) of the atmospheric parameters associated to the instants of the final selection, for every atmospheric data source (Default, AERONET,

⁷Notice from here on, the hat and the c will not be used anymore, for practicality purposes.

MODIS-AQUA, MERRA-2).

The model is run for the selected instants, with the corresponding air mass associated to the zenith angle, the seasonal reference atmosphere and atmospheric input parameters for all the atmospheric data sources (Default, AERONET, MODIS-AQUA, MERRA-2). The model outputs are then compared to their corresponding (matching time stamp) ground measurements of G_h , G_{dh} and G_b , and performance metrics are computed.

4.2.2. Different atmospheric inputs tested with SMARTS

Estimating clear sky spectral irradiance accurately requires detailed and precise information about the atmospheric state. When a data set of atmospheric parameters is integrated with the model's algorithms, it forms what is called a composite model. For example, SMARTS includes a default set of atmospheric parameters, thus when it is modelled with those parameters it creates the composite model: SMARTS + Default (here abbreviated as SM+DE). The description of the atmospheric state is then part of the composite model, and therefore any uncertainty or bias in the inputs will also impact the composite model performance.

In order to test different sources of atmospheric information typically available in this region, four atmospheric data sources will be tested to quantitatively determine the performance of each combined model. The sources of atmospheric information are: Default from SMARTS, AERONET, MODIS-AQUA and MERRA-2. Table 4.7 displays a summary of the parameters selected from each one, their temporal and spatial resolution, and the time delay until estimates are available online. Additional information regarding the exact name of the variables and the urls of access is presented in Table 4.8.

Table 4.6: Composite models abbreviations.

Description	Abbreviation
SMARTS smoothed + DEFAULT	SMs + DE
SMARTS smoothed + AERONET	SMs + AE
SMARTS smoothed + MODIS-AQUA	SMs + MO
SMARTS smoothed + MERRA-2	SMs + ME
SMARTS raw + DEFAULT	SM + DE
SMARTS raw + AERONET	SM + AE
SMARTS raw + MODIS-AQUA	SM + MO
SMARTS raw + MERRA-2	SM + ME

Some parameters need to be selected before SMARTS runs, regardless of the chosen composite model. Among these, the Reference Atmosphere (see Section 4.1). In this work, the Reference Atmosphere is chosen as Sub Tropical Summer (STS) or Sub Tropical Winter (STW), depending

Table 4.7: Summary of the data sources available for atmospheric parameters.

Source	Atmospheric Variable	Temporal resolution	Spatial Resolution	Uploaded after
AERONET	AOD ₅₀₀ , w, Ångström Exponent 440-870 nm	15-20 min (variable)	Local*	few days
MODIS AQUA	AOD ₅₅₀ , w	daily	1° × 1°	few days
MERRA-2	AOD ₅₅₀ , w, Ozone	hourly	0.5° × 0.625°	1-2 months
OMI	Ozone	daily	0.25° × 0.25°	few days

(*) The AERONET site is in Montevideo (Latitude: 34.91817°S, Longitude: 56.16677°W, altitude: 71.0 m), 500 km away from the site of interest in Salto.

Table 4.8: Summary of the variable names of each data source. The url's of access are: https://aeronet.gsfc.nasa.gov/new_web/units.html, <https://giovanni.gsfc.nasa.gov>.

Abbreviation	Description	Variable code
AERONET		
AOD ₅₀₀	Aerosol optical depth at 500 nm	AOD_500
$\alpha_{440-870}$	Ångström Exponent 440-870 nm	440-870_Angstrom_Exponent
w	Precipitable water vapor	Precipitable_Water(cm)
u_o	Total columnar ozone	Ozone(Dobson)
MODIS-AQUA		
AOD ₅₀₀	Aerosol optical depth at 550 nm	Aerosol Optical Depth 550 nm (Dark Target)
w	Precipitable water vapor	Precipitable Water Vapor-(IR Retrieval) Total Column
OMI		
u_o	Total columnar ozone	Ozone Total Column (TOMS-like)
MERRA-2		
AOD ₅₅₀	Aerosol optical depth at 550 nm	Total Aerosol Extinction AOT 550 nm
w	Precipitable water vapor	Total precipitable water vapor
u_o	Total columnar ozone	Total column ozone

on the season, STS is selected for spring and summer and STW is selected for winter and autumn. The Reference Atmosphere profiles of STW and STS require specifying the atmospheric pressure (P, hPa) and relative humidity (RH, %), which in this case have been set to the default values of $P = 1013.25$ hPa (for both STS and STW), $RH = 79.440\%$ for STW and $RH = 78.880\%$ for STS. Table B.4, included in Appendix B.10, lists the vertical profiles of temperature, atmospheric pressure, and relative humidity employed by SMARTS to define the STS and STW reference atmospheres.

In addition, all other atmospheric input variables that are not mentioned here or in Table 4.8, are considered of secondary importance and are left to their default values.

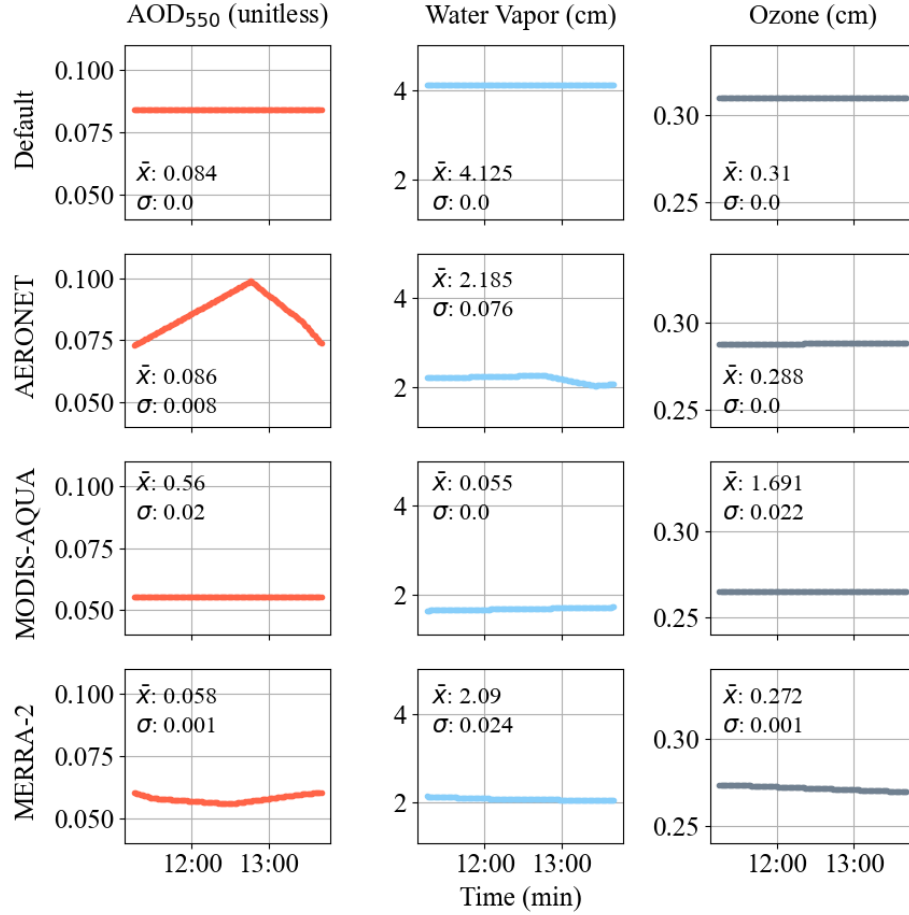


Figure 4.11: Time series of the atmospheric variables of the different data sources: Default, AERONET, MODIS-AQUA, MERRA-2 tested in SMARTS smoothed. Instants correspond to day 2024/06/18 around solar noon. The variables have been interpolated to 1-minute. $\bar{x}$ refers to the mean, and σ is the standard deviation. The maximum, minimum, mean and standard deviation values are shown in (Table C.2). Figure by Paola Russo.

The composite model SM+DE is run with Default atmospheric parameters as mentioned. They are suggested by SMARTS and will be used unless the user overrides them manually. Their values remain constant within a given run if the geographic coordinates and height of the place do not change, and the reference atmosphere selected remains fixed. For this reason, the default values for the parameters used here are constant throughout the whole period of study and

equal to: $\text{AOD}_{550} = 0.084$ (unitless), $w = 4.1252$ cm, $u_o = 0.3102$ cm. These parameters are plotted in Fig 4.11 for the instants used in the case of the spectral simulations. These values can also be contrasted with a larger period of data, such as the period used for the broadband simulation shown in Fig. C.1. The default SMARTS parameters should reflect typical clear-sky, mid latitude atmospheric conditions. An AOD_{550} of 0.084 represents low aerosol loading. A water vapour content of $w = 4.1252$ cm and an ozone column of $u_o = 0.3102$ cm should be similar to climatological averages for temperate zones, serving as a general baseline for radiative transfer simulations. However, in the case of water vapour, as Figure 4.11 shows, SMARTS default of 4.1252 cm is noticeably too high and more than twice the value of the estimates from the three other sources, which are about 2.0 cm.

The SMARTS plus AERONET composite model is named: SM+AE. SMARTS is going to be run for the location LES, Salto, but the closest AERONET site is in Montevideo (coordinates: -34.9182° , -56.1665° , 58 m.a.s.l.), located around 500 km of distance from Salto. This introduces inaccuracy due to spatial variability. However, testing SMARTS performance with ground measured inputs from a distant AERONET site is still considered to be relevant. The atmospheric parameters used from AERONET are: AOD_{500} , Ångström exponent at 440-870 nm, precipitable water vapour, w , and total ozone column, u_o . AOD_{550} (the actual input used by SMARTS) is inferred from the AOD_{500} and Ångström exponent (Eq. 2.24). AERONET data during the test day was very sparse, furthermore the estimates are separated by time intervals of varying length. Thus for usability purposes, the data are interpolated at 1 minute intervals. As shown in Table 4.7, some data sources can have a delay of months before they become available online. AERONET data is available within a few days.

The SMARTS plus MODIS composite model (SM+MO) uses data from MODIS, which has been described in Section 2.4. Spectral measurements for this work have been taken around noon, where both MODIS satellites (AQUA and Terra) have a good coverage of Uruguay. Either of them would provide useful data, in this case, the Aqua satellite has been selected. The products that will be used from MODIS-AQUA are AOD_{550} , and w , as shown in Table 4.7. These products are provided as daily averages, since the satellite makes two daily passes over any given point on the surface (one during daytime and one during night time). Therefore a linear interpolation is applied to obtain data at the required one-minute intervals. The data are available for download only a few days after the spectral irradiance measurement has been done, which represents an advantage from this data source compared to MERRA-2. For this composite model the remaining variable, u_o , is extracted from OMI (discussed in Section 2.4).

The SMARTS plus MERRA-2 composite model is SM+ME. The variables used from MERRA-2 are: AOD_{550} (unitless), w (kg/m^2), u_o (DU). All units are converted to cm as required by SMARTS: w (cm) = w (kg/m^2) $\times 0.10$ and u_o (cm) = u_o (DU) $\times 10^{-3}$.

The values of the atmospheric parameters during the instants selected for each data source are shown in Fig. 4.11. These plots are complemented by Table C.2, in Appendix C.2, presenting

more details such as maximum, minimum and mean values. In what follows, the composite models will be abbreviated as shown in Table 4.6. Notice letter s will be used to differentiate smoothed from raw.

4.3. Results

4.3.1. Sensitivity of SMARTS to relevant input parameters

A simple sensitivity analysis is performed, to quantify how sensitive the model is to changes in the atmospheric parameters. The model will be tested with a specific value for AOD_{550} , w and u_o . Next, each variable will be varied in turn, leaving the others fixed in order to see how much the estimated spectral irradiance changes. This will support the understanding of the conclusions in the last section of this chapter.

The selected sample instant is day 2022-01-11 12:00 (UTC-3) in Salto. Using the selected specific atmospheric input values for AOD, w , and u_o , a nominal spectra ($G_{b,\lambda}^n$) is obtained. The selected instant has been arbitrarily chosen and corresponds to a spring day, independent from the period of the rest of the study. This day is known to be of clear sky and stable atmospheric conditions.

In what follows, one input variable (called generically x_0) is varied by 60% (an arbitrarily selected percentage) and two new beam spectra (one greater, $G_{b,\lambda}^+$, corresponding to a decrease in x_0 , and one smaller, $G_{b,\lambda}^-$, corresponding to an increase in x_0) are generated with input values:

$$x_{\pm} = x_0 \pm \Delta x = x_0 \left(1 \pm \frac{\Delta x}{x_0} \right) \quad \text{with } \Delta x/x_0 = 0.6. \quad (4.20)$$

The chosen nominal values are: $\text{AOD}_{550} = 0.131$, $w = 1.86$ cm and $u_o = 0.256$ cm. These values correspond to MERRA-2 data for that moment. Then AOD_{550} is decreased to $\text{AOD}_{550} = 0.052$, while w and u_o remain constant, and next, AOD_{550} is increased to $\text{AOD}_{550} = 0.209$ while leaving w and u_o fixed. The procedure is replicated for the other two parameters obtaining the nominal and extreme values shown in Table 4.9. The last row of Table 4.9 shows the sensitivity of SMARTS to air masses in the range of 1.50 and 2.00⁸.

Once the model is run using these inputs, the corresponding relative changes in the SMARTS spectra are quantified as a % of the integrated nominal spectrum,

$$\delta G_b^{\pm} = 100 \times \frac{\int_{280 \text{ nm}}^{4000 \text{ nm}} \left(G_{b,\lambda}^{\pm} - G_{b,\lambda}^n \right) d\lambda}{\int_{280 \text{ nm}}^{4000 \text{ nm}} G_{b,\lambda}^n d\lambda}. \quad (4.21)$$

⁸These values have been arbitrarily selected, they do not correspond to the nominal $m \pm 60\%$ because decreasing the nominal value a 60% would return 0.417 which is a physically impossible air mass.

Table 4.9: Sensitivity of SMARTS to changes in input variables, for instant 2022/01/11 at 12:00 (UTC-3), Salto. $G_{b,\lambda}^+$ corresponds to a decrease in x_0 , and $G_{b,\lambda}^-$ corresponds to an increase in x_0 . The spectral variation δG_b is calculated with Eq. (4.21).

Variable	nominal (x_0)	low (x^-)	high (x^+)	$G_{b,\lambda}^+$	$G_{b,\lambda}^-$	δG_b^+ (%)	δG_b^- (%)
AOD ₅₅₀	0.131	0.052	0.209	1021.9	906.1	5.7	-6.3
w (cm)	1.862	0.744	2.980	1001.3	937.4	2.5	-4.2
u_o (cm)	0.256	0.102	0.410	966.5	956.9	0.5	-0.5
m	1.042	1.500	2.000	863.7	775.4	-10.2	-19.3

The results of this procedure are shown quantitatively in Fig. 4.12 and Table 4.9. Smaller AOD₅₅₀ values, Fig. 4.12(a), tend to increase the modelled spectral irradiance, particularly in the visible range, 400-700 nm, as expected. A higher concentration of water vapour reduces spectral irradiance, Fig. 4.12(b), particularly at the known water vapour absorption bands in the near infrared (820 nm and 900-1000 nm) Dubuisson et al. (2004). Meanwhile, a decrease in ozone concentration slightly increases the spectral irradiance at short wavelengths, Fig. 4.12(c), as expected.

To understand the results of the sensitivity analysis, consider Fig. 4.12 as an example. When AOD₅₅₀ is varied by $\pm 60\%$, it results in a δG_b of $\pm 6\%$, while varying w and u_o results in δG_b values of $\pm 3\%$ and $\pm 0.5\%$, respectively. This suggests that AOD₅₅₀ is the most influential variable affecting the intensity of $G_{b,\lambda}$, and ozone is the least influential, within the wavelength range of 300–1100 nm, among the variables tested. But, a question that arises, is: what changes in $G_{b,\lambda}$ could be expected from real variations of these parameters? do real variations resemble the ones tested here?. For this purpose, complementary information is added to the discussion. Consider the maximum and minimum values of AOD₅₅₀, w and u_o from the previous 5 years shown in Fig. C.1. Take as an example w , its values have typically fluctuated between 1 to 5 cm (under clear sky conditions lower values are to be expected). In this case, the variations tested in the sensitivity analysis (changes of 60 % in 1.86) are quite small in terms of w , meaning the increases or decreases that are going to be observed in $G_{b,\lambda}$ under typical atmospheric fluctuations will likely be magnified. In the case of AOD, with typical variations in the order of 1.000, the typical atmospheric fluctuations will produce similar results to those observed in this sensitivity analysis. However, u_o usually tends to fluctuate in smaller orders, for example, its values have been between 0.270 and 0.310 cm during the last 5 years, thus the variations tested in this sensitivity analysis (60 % of 0.256) are overdimensioned, and the variations expectable of $G_{b,\lambda}$ due to u_o atmospheric fluctuations will be much smaller. In overall, the typical variations of this three parameters in real atmospheric conditions, amplify the effects described in δG_b .

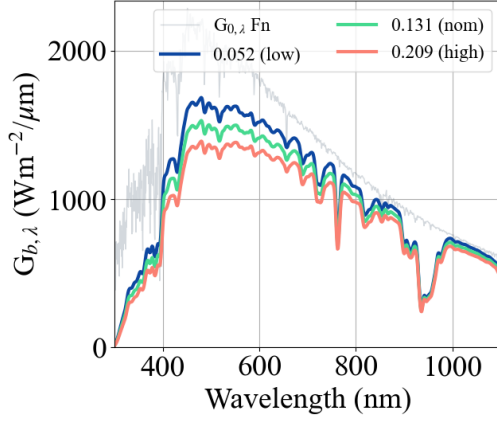
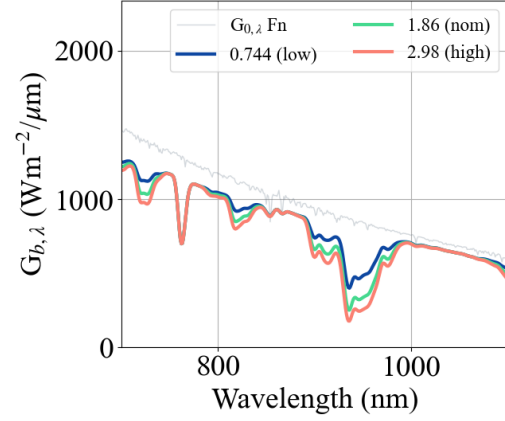
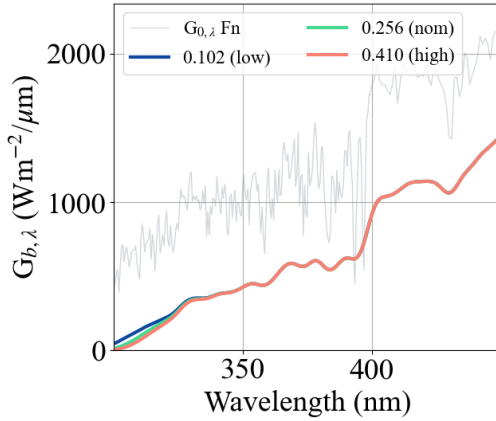
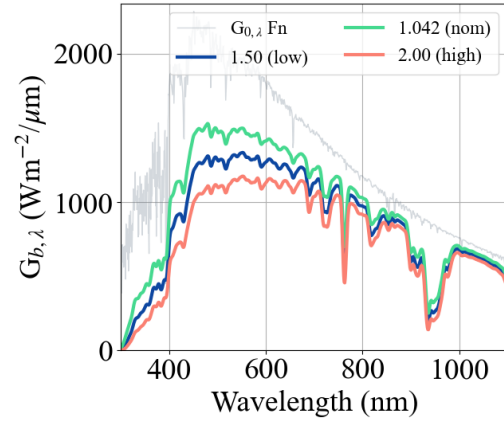
(a) AOD₅₅₀(b) water vapour, w (cm)(c) Ozone column, u_o (cm)(d) Air mass, m (cm)

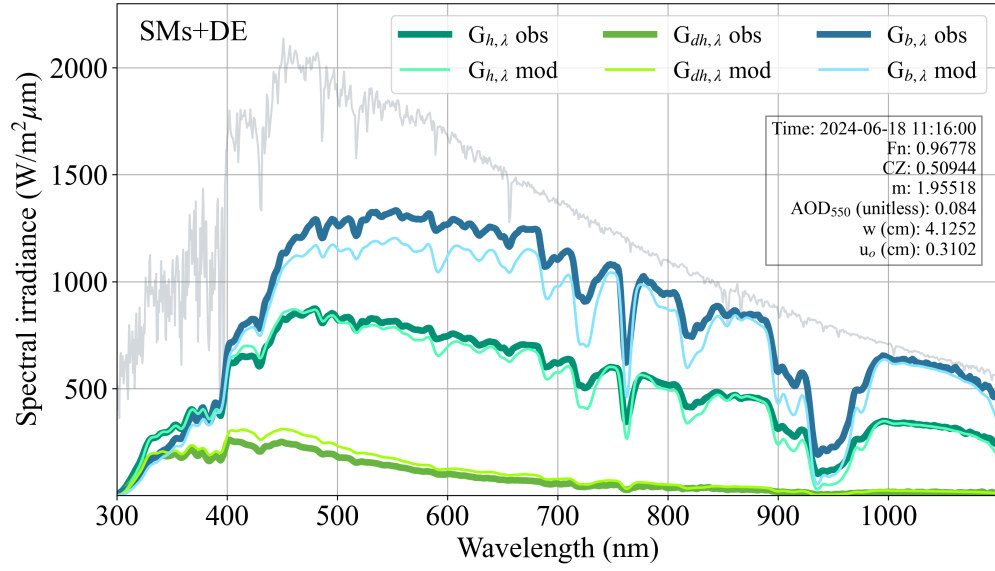
Figure 4.12: Sensitivity of SMARTS smoothed to changes in the input parameters: AOD₅₅₀, w and u_o , zoomed in the spectral region of main influence of each parameter. The abbreviations correspond to: nom - nominal value tested, high - upper value, low - lower value. The grey spectrum corresponds to irradiance at the top of the atmosphere (Gueymard, 2004) corrected by the sun earth distance correction factor, and it is shown as a reference. Figure by Paola Russo.

4.3.2. Performance of SMARTS spectral estimates

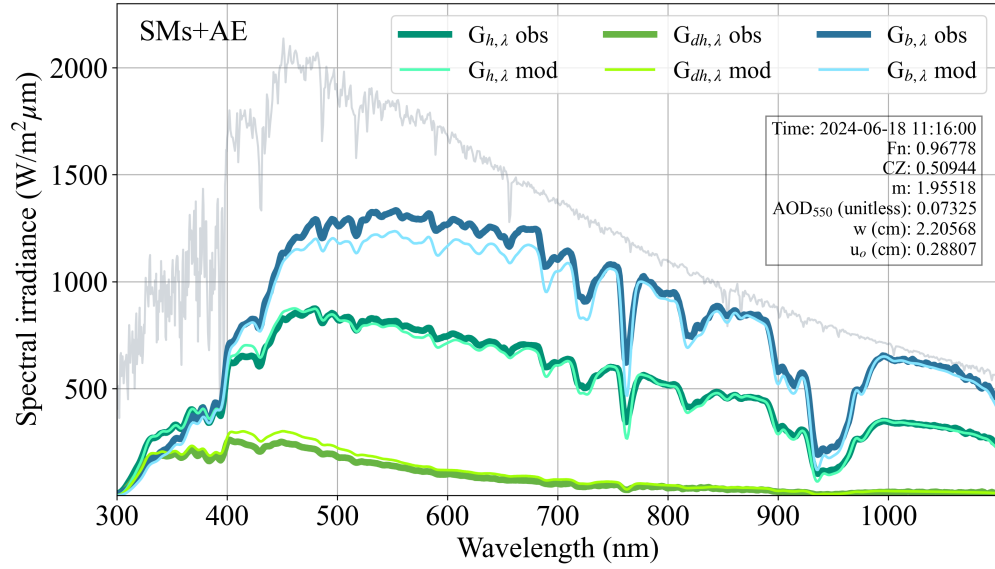
Figure (4.13) and Figure (4.14) show the spectral results of SMARTS for its products: $G_{h,\lambda}$, $G_{dh,\lambda}$ and $G_{b,\lambda}$, at a sample instant. Bold dark lines correspond to observed spectra, while thin light lines represent modelled spectra using different atmospheric data sources. Overall, the three products are well modelled: $G_{h,\lambda}$ shows consistently good performance throughout the spectrum, whereas $G_{b,\lambda}$ presents slightly larger discrepancies, which are transferred to $G_{dh,\lambda}$ in the PAR region, particularly between 400-500 nm. The residuals appear to be partially related to the atmospheric input variables (Figs. 4.13, 4.14 and 4.16), since for the same instant and equal conditions, the models exhibit different residual magnitudes depending on the atmospheric data source. The largest absolute residuals occur in $G_{b,\lambda}$, while $G_{dh,\lambda}$ and $G_{h,\lambda}$ show smaller residuals.

By visual inspection, the composite models are ranked from best to worst as SMs+MO, SMs+ME, SMs+AE, and SMs+DE. SMs+MO (Fig. 4.14) reproduces the measured irradiances accurately over most of the spectrum, with only minor discrepancies near the PAR region, particularly in the beam component, which is primarily influenced by AOD. Regarding water vapour, SMs+MO shows better performance, as it accurately reproduces the absorption bands (e.g., around 935 nm). Errors appear in the O₂ absorption feature near 760 nm, which is expected since this parameter was kept at its default value. The increase in error among composite models is related to uncertainties in the atmospheric parameters; consequently, SMs+ME performs better than SMs+AE, and both outperform SMs+DE. Although AERONET estimates are derived from high precision ground-based retrievals, SMs+AE shows poorer results due to additional uncertainty caused by spatial variability, as the station is located approximately 500 km from the modelled site. SMs+DE exhibits the worst performance, likely due to the use of time-invariant parameter values that differ substantially from satellite and reanalysis estimates (Table C.2, Fig. 4.11). For example, w is fixed at about 4.0 cm, compared to average values near 2.0 cm from MODIS and MERRA-2; similarly, AOD₅₅₀ and u_o are overestimated. These discrepancies indicate that the default parameters do not adequately represent the local atmospheric conditions, both because they fail to capture the natural temporal variability of the atmosphere and because their values are not adapted to the local climatic conditions.

The relative metrics (as shown in Table 4.10) are adequate for a comparison between $G_{h,\lambda}$, $G_{dh,\lambda}$ and $G_{b,\lambda}$, since relative values are independent of the mean observed irradiance intensity, which is different in every product. In the UV spectral range the best product modelled is $G_{h,\lambda}$, then comes Beam and the worst is $G_{dh,\lambda}$. This behaviour is replicated at all the spectral ranges tested (UV, PAR, NIR, EKO), for every composite model, except for SM+DE and SMs+ME specifically in the NIR range, where the order of best performing product is: Global, Diffuse and Beam. The Default value for precipitable water vapour (see Appendix C.1 and Fig. 4.11) is 4.125 cm, almost one half of the estimated values by MODIS-AQUA which is 2.089 cm. This means the composite model SMs+DE will present a larger underestimation than the other composite models, mainly in $G_{b,\lambda}$. This explains why the order of performance of the products switches to $G_{h,\lambda}$, $G_{dh,\lambda}$ and $G_{b,\lambda}$, since the estimation of Beam is poor due to the misrepresentation of w .

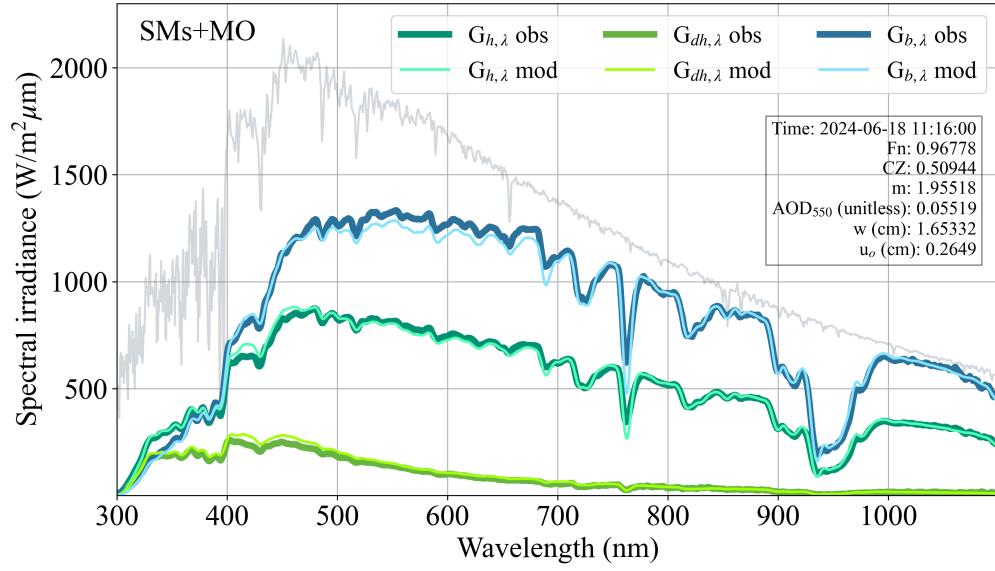


(a) SMs+DE

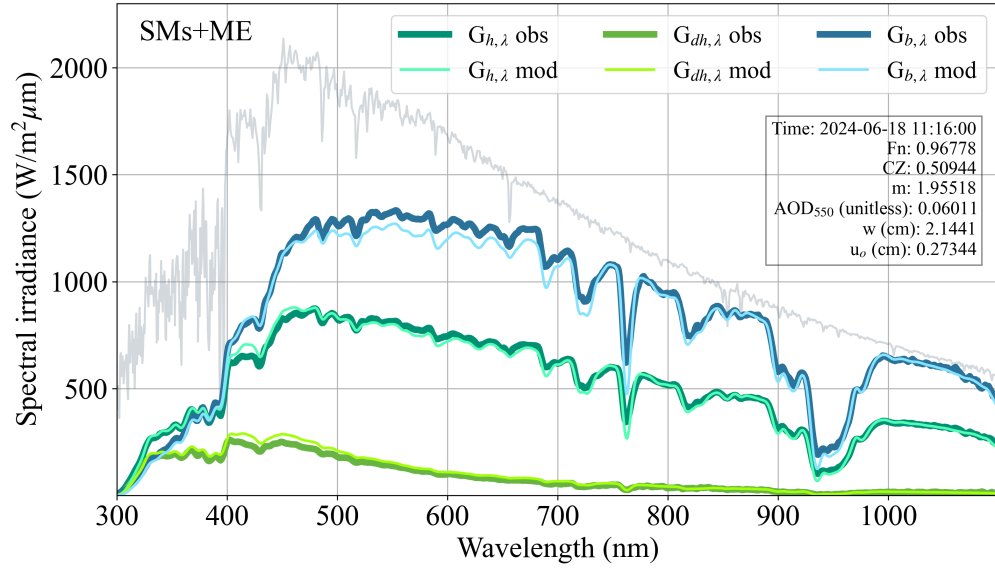


(b) SMs+AE

Figure 4.13: Spectral irradiance vs. wavelength of modelled (SMs+DE, SMs+AE) and observed Global, Diffuse and Beam. Figure by Paola Russo.



(a) SMs+MO



(b) SMs+ME

Figure 4.14: Spectral irradiance vs. wavelength of modelled (SMs+MO, SMs+ME) and observed Global, Diffuse and Beam. Figure by Paola Russo.

Figure 4.15 shows MBD in absolute terms plus and minus RMSD, for the three products: global (oranges), diffuse (greens) and beam (blues), for every composite model tested. This information is discriminated by wavelength range: 300-400 nm (UV), 400-700 nm (PAR), 700-1100 nm (NIR) and 300-1100 nm (band measured by EKO instrument). In support of this figure, Table 4.10 offers the values in relative terms. It can be observed again that SMs+MO outperforms all the other composite models, in almost every wavelength range, and almost every component (with the exception of the NIR band of the diffuse component). This coincides with the results over broadband irradiance (addressed in the next section, supporting the explanations presented).

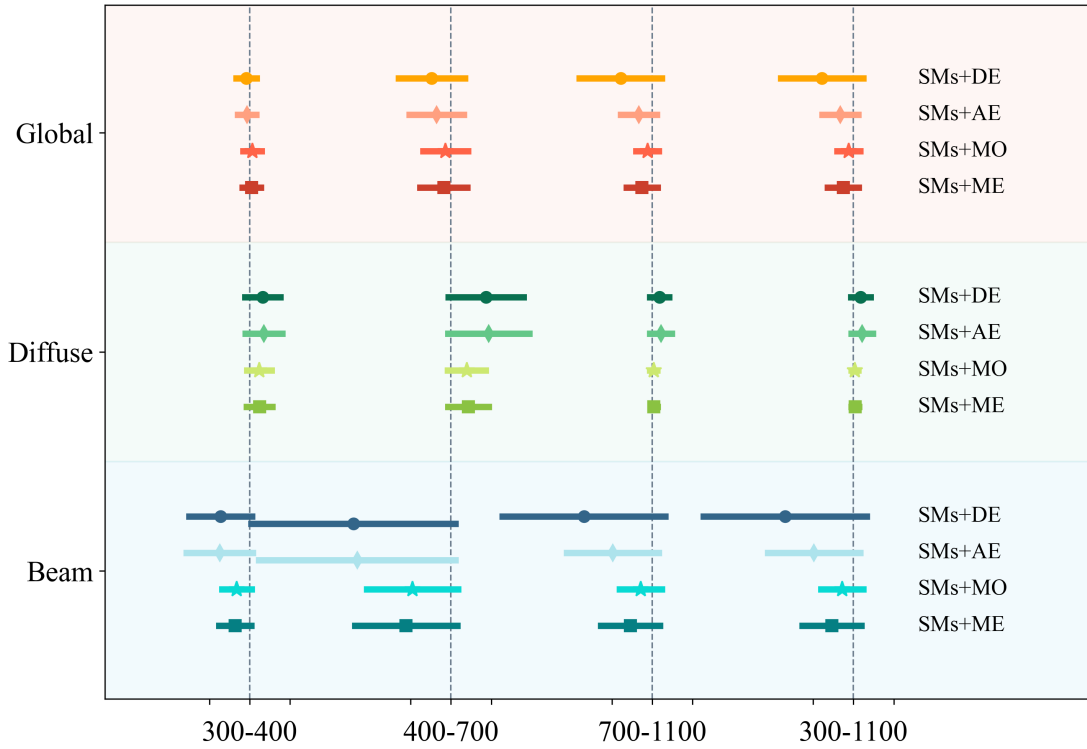


Figure 4.15: MBD $\pm$ RMSD for the bands 300-400, 400-700, 700-1100 and 300-1100 nm, for every product: Global (Orange), Diffuse (Green) and Beam (Blue), for different composite models: SMs+DE (being the MBD shaped with a circle), SMs+AE (diamond), SMs+MO (star), SMs+ME (square). (In 400-700 nm default and AERONET lines have been moved down for visualization purposes). The dotted lines are axis origins ($0 \text{ W/m}^2\mu\text{m}$) for each spectral range, and the marks in the x axis denote minus and plus $50 \text{ W/m}^2\mu\text{m}$. Figure by Paola Russo.

Another pattern observed in the performance by spectral regions (Table 4.10) is that SMs+MO seems the least biased in the products $G_{h,\lambda}$, $G_{dh,\lambda}$ and $G_{b,\lambda}$, for each wavelength range (UV, PAR and NIR).

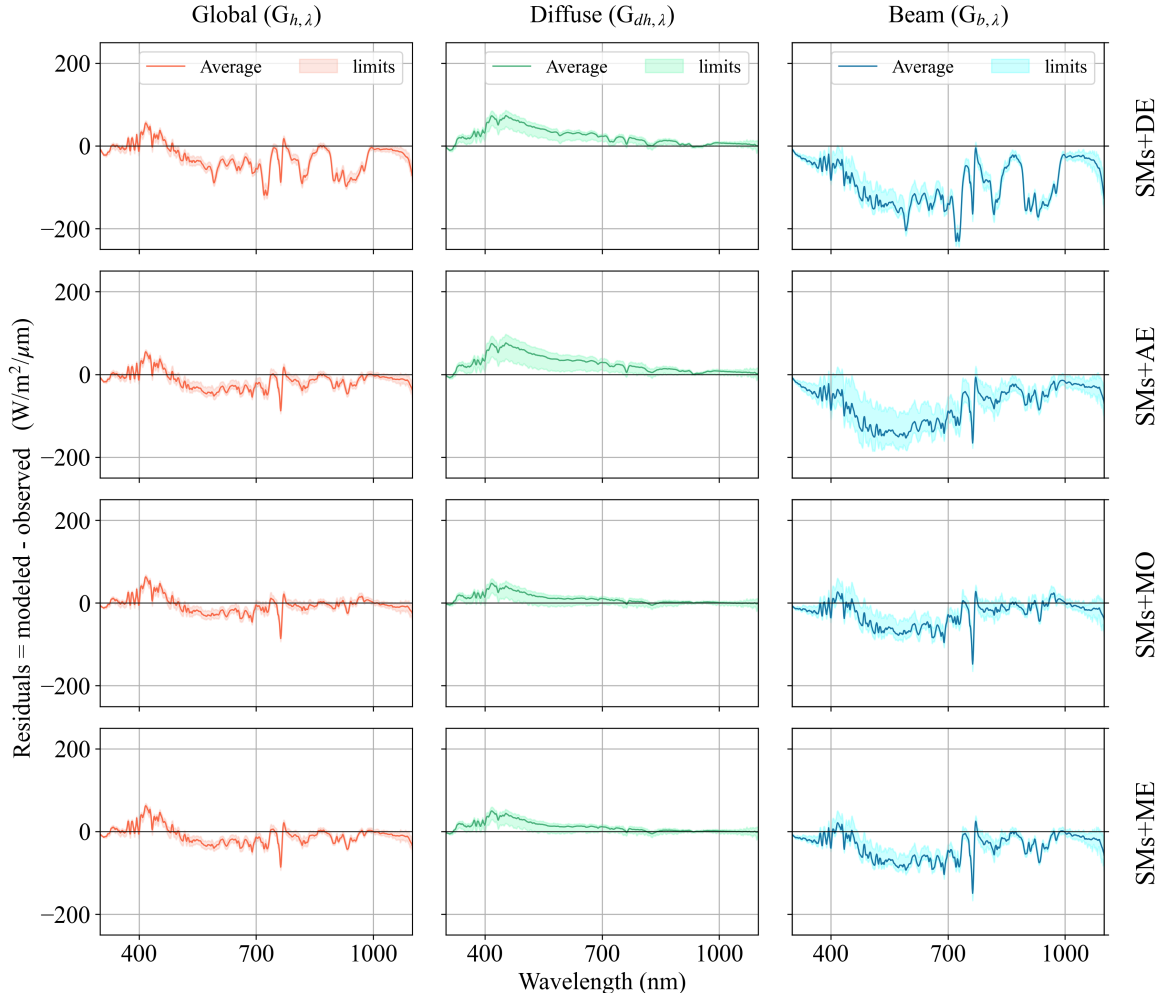


Figure 4.16: Spectral differences between model and measurements. The line represents the mean, while the shaded band shows the maximum and minimum differences during the period analyzed. Figure by Paola Russo.

The residuals in Fig. 4.16, calculated as modelled minus observed (note that the integral of the residuals corresponds to the MBD), provide information on the spectral distribution of errors. SMs+DE exhibits a large negative bias in $G_{h,\lambda}$ and $G_{b,\lambda}$ across the entire spectral range, which progressively decreases from SMs+AE to SMs+ME and SMs+MO, the latter showing the smallest residuals. For the beam component, the negative bias mainly affects the PAR region, the water vapour absorption bands, and the feature around 760 nm. This underestimation may be caused by model parameterizations or by overestimated atmospheric inputs, such as water vapour in the Default composite model. The discrepancy around 1100 nm should not be considered, as measurements near the instrument's spectral limit are affected by high uncertainty.

Observing the residuals for the diffuse component, the curve looks close to zero in the y-axis, but it should be kept in mind that looking at it in absolute terms is not fair, because the diffuse is a small fraction of beam or global irradiance. It also has a healthy balance between negative and positive bias, but for the small bump near 450 nm. As mentioned before, Global in SMARTS is calculated from closure using the other two components, thus opposite biases in beam and diffuse are cancelling each other, yielding a low bias in global irradiance. Still, the observations made upon the Beam are predominant because its intensity is much larger than that of the diffuse.

Observing the main region of influence of water vapour (around 935 nm) in Figs. 4.13 and 4.14 the data source MODIS-AQUA has the best accuracy. This is also supported by the quantitative result of MBD and RMSD in the 700-1100 nm region, shown in Tab. 4.10. Following them in decreasing accuracy, there are MERRA-2 and AERONET, and the least accurate is Default. On the other hand, the variable AOD₅₅₀ still needs further research, since the performance in its main region of influence (PAR) shows a negative bias and even though it is small, it still leaves room for improvement. If the negative bias turned out not to be caused by an inaccuracy in AOD₅₅₀ then other options could be tested, such as for example Tropospheric Nitrogen Dioxide (NO₂), which at first was not considered here but since it acts in the region 320-700 nm (Vasilkov et al., 2009), it could be interesting to test if it makes a visible improvement. Ozone on the other hand, seems to be accurate enough, as the model performed reasonably well in the UV-A region, which is as far as the instrument allows the comparison.

The broadband performance of the model specifically in the 300-1100 nm region is shown as dispersion plots in Fig. 4.17⁹. These plots show the integral of the composite model's global (and its components) vs. the corresponding integrated observations. An interesting pattern of a boomerang appears in Global, Diffuse and Beam. This is not an issue of the measurement instrument, since the pattern appears both, when the integral of the model is compared against the integral of the spectroradiometer measurements (Fig. 4.17), and when it is compared against independent pyranometer and pyrhelimeter measurements (Fig. C.3). The pattern is observed in intraday temporal scale, and when a much larger sample is observed, it is not distinguishable, as in Fig. 4.18. The pattern could be related to changes in the accuracy of the atmospheric parameters in an intraday scale, however, the fact that it appears in all the composite models, suggests that it is independent of the atmospheric source. Another possibility is that it could be related to undesired effects of the model structure, maybe related to the aerosol parametrization or the treatment of diffuse and direct irradiance. Further tests will need to be done in the future.

⁹Note that this differs from the broadband comparison made in the next section, because it uses the smoothed spectral output integrated in range of the spectroradiometer (300-1100 nm), while the one discussed in the next section uses SMARTS raw outputs, integrated in 280-4000 nm, which can be compared to pyranometer or pyrhelimeter measurements in the 300-3000 nm range

Table 4.10: Performance metrics (Eq. 2.28) for SMs+DE, SMs+AE, SMs+MO, SMs+ME, per wavelength range. The MBD and RMSD are expressed in relative terms (rel, %) and absolute terms (abs, $\text{W/m}^2/\mu\text{m}$) and the observed mean in ($\text{W/m}^2/\mu\text{m}$).

		Wavelength range (nm)							
		300-400		400-700		700-1100		300-1100	
		abs	rel	abs	rel	abs	rel	abs	rel
Global horizontal ($G_{h,\lambda}$)									
SMs+DE	MBD	-4.1	-0.7	-23.8	-4.1	-39.1	-6.8	-28.9	-5.0
	RMSD	12.5	2.2	41.1	7.2	51.2	8.9	44.3	7.7
SMs+AE	MBD	-3.3	-0.6	-17.9	-3.1	-16.5	-2.9	-15.4	-2.7
	RMSD	11.3	2.0	33.8	5.9	22.4	3.9	26.4	4.6
SMs+MO	MBD	3.2	0.6	-6.7	-1.2	-5.9	-1.0	-5.1	-0.9
	RMSD	11.5	2.0	27.9	4.9	14.1	2.4	20.2	3.5
SMs+ME	MBD	2.4	0.4	-9.0	-1.6	-12.7	-2.2	-9.4	-1.6
	RMSD	11.5	2.0	29.4	5.1	19.2	3.3	22.9	4.0
Mean Obs		322.0		843.7		435.7		574.1	
Diffuse horizontal ($G_{dh,\lambda}$)									
SMs+DE	MBD	16.0	17.7	43.5	48.1	9.0	8.1	22.4	24.8
	RMSD	21.9	24.2	46.6	51.6	12.0	10.9	30.6	33.8
SMs+AE	MBD	17.4	19.3	46.9	51.9	10.8	11.9	25.1	27.8
	RMSD	22.8	25.2	50.5	55.8	13.4	14.8	33.3	36.8
SMs+MO	MBD	11.9	13.2	19.6	21.7	1.7	1.9	9.7	10.7
	RMSD	15.4	17.1	23.5	26.0	4.4	4.9	15.7	17.4
SMs+ME	MBD	12.2	13.5	21.7	24.0	2.1	2.3	10.7	11.8
	RMSD	15.9	17.6	25.2	27.9	4.6	5.1	16.8	18.6
Mean Obs		165.9		151.1		26.2		90.4	
Beam normal ($G_{b,\lambda}$)									
SMs+DE	MBD	-36.3	-4.2	-121.2	-14.0	-84.8	-9.8	-92.3	-10.7
	RMSD	39.1	4.5	126.8	14.7	101.2	11.7	106.4	12.3
SMs+AE	MBD	-37.3	-4.3	-116.4	-13.5	-49.0	-5.7	-72.8	-8.4
	RMSD	41.1	4.8	122.0	14.1	57.2	6.6	86.2	10.0
SMs+MO	MBD	-16.0	-1.9	-47.9	-5.5	-14.1	-1.6	-27.0	-3.1
	RMSD	18.3	2.1	56.6	6.6	26.1	3.0	39.8	4.6
SMs+ME	MBD	-17.9	-2.1	-55.8	-6.5	-27.0	-3.1	-36.6	-4.2
	RMSD	20.0	2.3	63.6	7.4	36.7	4.2	47.3	5.5
Mean Obs		278.5		1236.2		731.0		863.3	

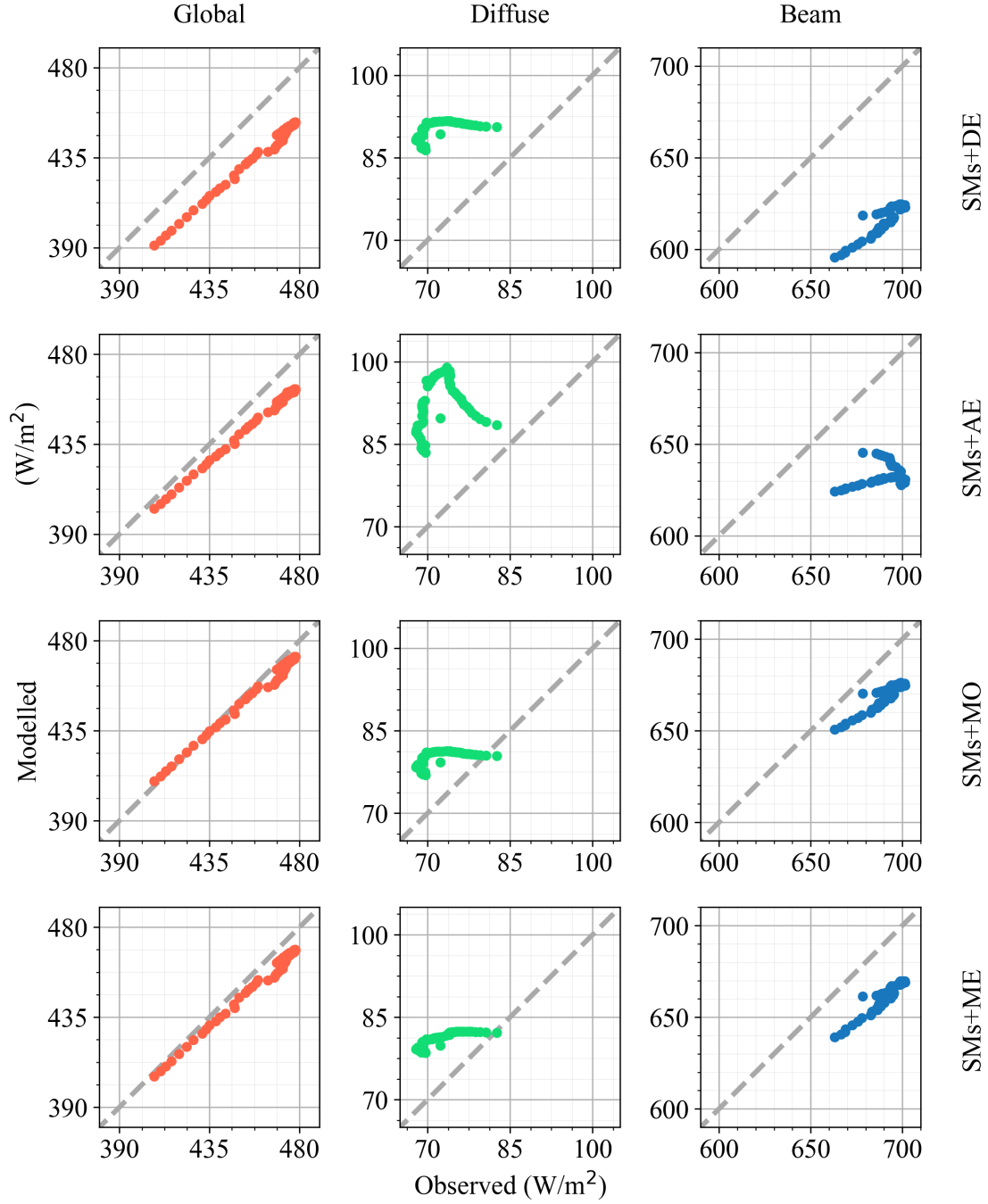


Figure 4.17: Scatter plots comparing SMARTS spectral irradiance integrated (300-1100 nm) with EKO measurements of Global ($G_{h,\lambda}$), Diffuse ($G_{dh,\lambda}$) and Direct ($G_{b,\lambda}$) integrated in the same spectral range. See Fig. 4.11 and Table 4.10 for details on the input parameters and performance metrics, respectively. Note that different scales are used for the different variables. Figure by Paola Russo.

Spectral uncertainty

The calibration uncertainty of EKO MS-711 N is not provided by the manufacturer, however, it is important to estimate its value, since it provides a lower limit for the precision of the model that it is possible to evaluate from the instrument's measurements. For this reason, in Appendix C.4, the guidelines JCGM (2008) have been applied to estimate the instrument uncertainty of the spectroradiometer (μ_g , μ_d , μ_b), for each setup of the instrument ($G_{h,\lambda}$, $G_{dh,\lambda}$ and $G_{b,\lambda}$). It is known that spectroradiometers have varying uncertainty depending on the wavelength, however, since this is an analytic estimation, not an empirical calibration, this variations will be neglected. The results have been summarized in Table 4.11. The instrument uncertainties in

Instrument measuring	$G_{h,\lambda}$	$G_{dh,\lambda}$	$G_{b,\lambda}$
μ (W/m ² μ m)	21.8	21.8	30.9

Table 4.11: Expanded uncertainty, μ .

each product, μ_g , μ_d , μ_b are compared to the performance results of the model (RMSD) shown in Table 4.10. It is observed that the best model, SMs+MO, presents approximately equal or lower dispersions than μ_g and μ_d , in almost all the wavelength ranges, this means that the model has a precision similar to that of the instrument (for evaluating less dispersion, a more precise instrument should be used). $G_{b,\lambda}$ is the only product exhibiting a high dispersion (RMSD = 56.6 W/m² μ m), when compared to the instrument's uncertainty ($\mu_b = 30.9$ W/m² μ m) in the PAR region (400–700 nm). This behaviour may arise from limitations in the model algorithms and/or from uncertainties propagated through the atmospheric input parameters. Consequently, there is potential for further improvement in this product.

4.3.3. Performance of SMARTS broadband irradiances

SMARTS provides raw spectral irradiance, which integrated in the 280–4000 nm region, become the broadband irradiance estimates of the magnitudes G_h , G_{dh} and G_b . These can be compared to measurements of pyranometers and pyrhemimeters.

Figure 4.19 shows a quantitative representation of the MBD and RMSD in absolute terms, supported by Table 4.12 showing their corresponding relative indicators, rMBD and rRMSD (%). Ordered from best to worst performance, the results are: SM+ME and SM+MO with very similar results, then SM+AE and SM+DE. This is aligned with the results obtained spectrally, and can also be explained by similar reasons.

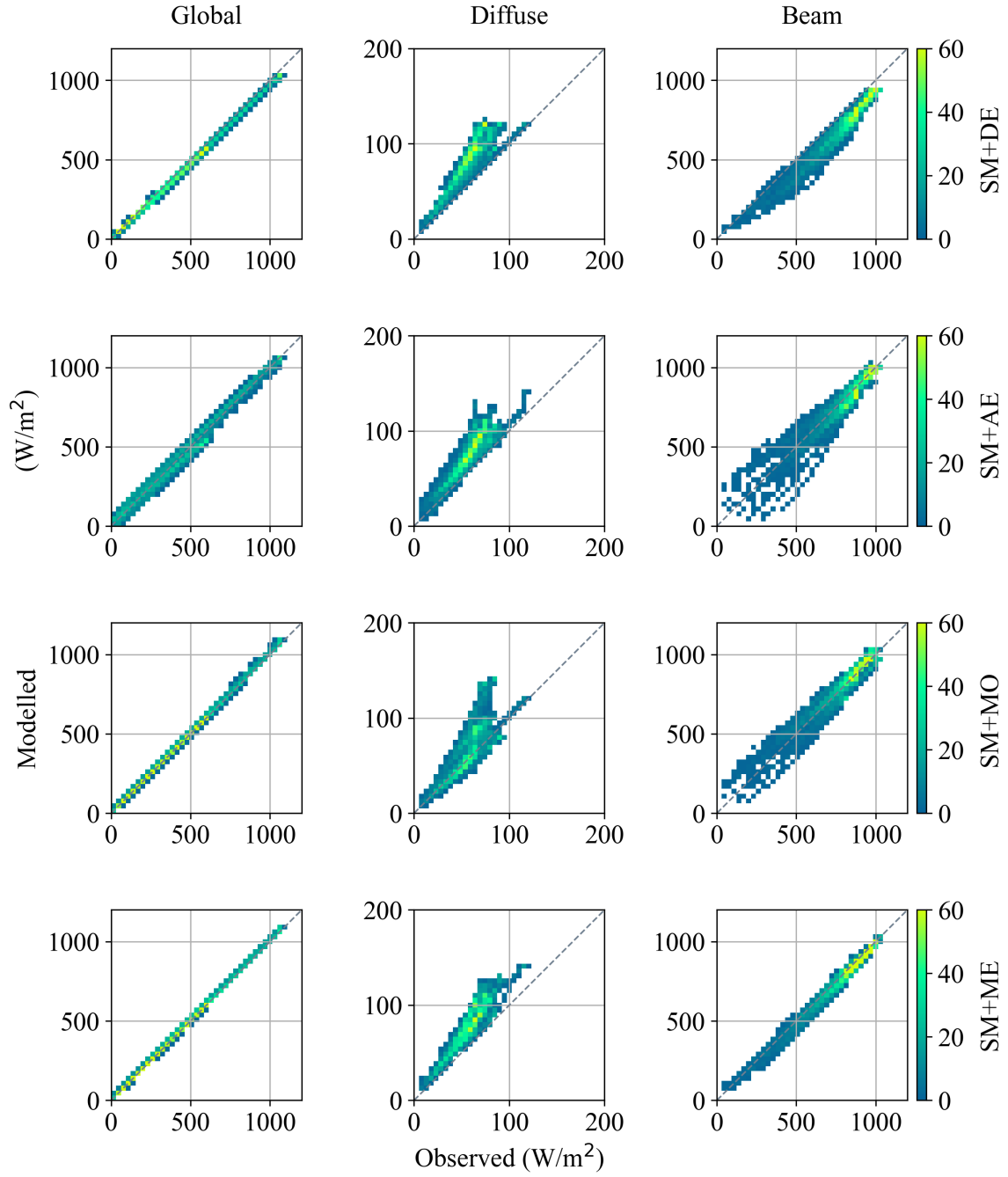


Figure 4.18: Scatter plots of SMARTS (integrated in 280-4000 nm) vs. broadband measurements. Plotted 2249 instants, selected from the period 2020/01/01 to 2024/12/31, originally from 1 minute samples during clear-sky and stable atmospheric conditions. Samples include 28 days equally distributed between seasons and zenith angles. The corresponding performance values are presented in Table 4.10. Figure by Paola Russo.

As a first general result observed, there is an underestimation in G_b and an overestimation in G_{dh} , particularly at high irradiance values (Fig. 4.18). The biases cancel out partially in G_h . This happens markedly for some atmospheric sources, although the effect is smaller for SM+ME and absent for SM+MO (which shows small positive bias). This suggests that it is associated to the quality of the atmospheric info.

Table 4.12: Performance metrics of the SMARTS composite models (integrated over 280-4000 nm). MBD and RMSD are presented in absolute terms (abs, W/m^2) and relative terms (rel, %) as percentage of the observed mean (last row, in W/m^2). Fig. 4.19 represents these results. Based on 2249 samples.

Atmos. data	Metric	G_h		G_{dh}		G_b	
		abs	rel	abs	rel	abs	rel
SM+DE	MBD	-19.4	-4.1	24.3	40.9	-86.4	-11.2
	RMSD	23.5	4.9	27.4	46.6	96.0	12.4
SM+AE	MBD	0.0	0.0	18.0	30.4	-14.4	-1.9
	RMSD	35.3	7.4	21.3	35.9	65.5	8.5
SM+MO	MBD	7.5	1.6	12.0	20.2	5.7	0.7
	RMSD	12.0	2.5	22.1	37.3	52.1	6.7
SM+ME	MBD	8.0	1.7	21.1	35.4	-18.1	-2.4
	RMSD	10.3	2.2	23.8	40.1	32.5	4.2
Mean Obs		476.8		59.4		772.0	

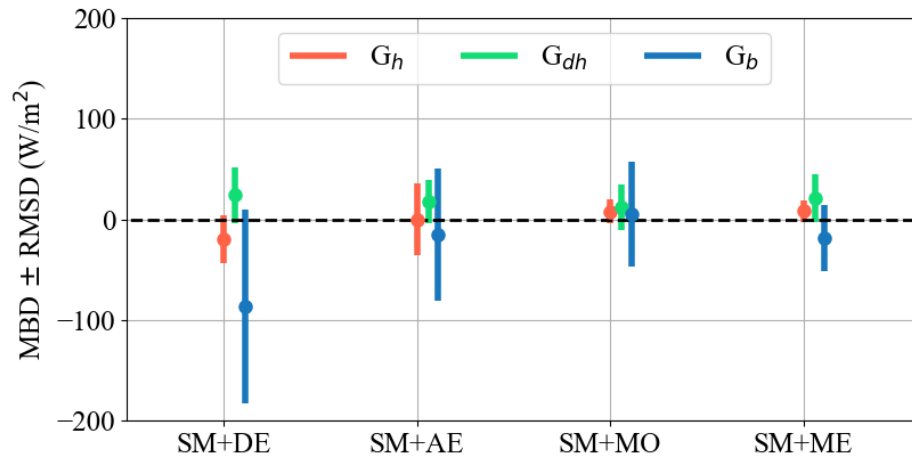


Figure 4.19: Broadband performance of the composite model variants (horizontal axis) for G_h (orange), G_{dh} (green) and G_b (blue). The corresponding numeric values are shown in Table 4.12. Figure by Paola Russo.

The best performances in G_h and G_{dh} are from SM+MO, with a bias of 1.6 % and 20.2 % respectively (relative to a mean of 476.8 and 59.4 W/m²). SM+ME has the best performance in G_b with a bias of -2.4 % (relative to a mean of W/m²). Even though SM+AE has a perfect bias for G_h , its RMSD is slightly higher. Regarding dispersion, SM+ME has the best dispersion in G_h and G_b , with an RMSD of 2.2 % and 4.2 %. SM+AE has the best dispersion in G_{dh} . At the same time, SM+MO is very close to SM+ME. The worst results were always from SM+DE. The results in G_h and G_b are considered to be good, taking into account that a typical broadband radiometer has an uncertainty of approximately 1.0 %, thus they are close to the instrument's uncertainty.

To understand these results, it is necessary to integrate the prior knowledge presented about how the model works and also about the characteristics of each atmospheric input (see Section 4.1 and Section 2.4).

Regarding the results of G_b , which is the first variable SMARTS calculates, the reason for the performance results can be related to the atmospheric inputs and their precision in the instants modelled. AERONET gives a large dispersion and some bias because their atmospheric inputs include a large spatial uncertainty since the station is far away from the point modelled. The bias of SM+MO is small, 0.7 %, indicating that the atmospheric parameters from MODIS were accurate in this site and what is transferred into accuracy of the model. However, SM+MO shows more dispersion than SM+ME, that can be explained because it is a retrieval from satellite measurements, that have more accuracy during the moment where the satellite passes by the site and less during the rest of the time. This is supported by the spectral results obtained in Fig. 4.14 where it can clearly be observed how some instants have a high accuracy with SMs+MO and a little bit less with SMs+ME. This hypothesis is also supported by Fig. C.3 and Table C.6 from Appendix C.5, where the broadband results of a single day are isolated, to be observed in detail.

The next product that is directly calculated by SMARTS is G_{dh} . In this case it is observed that all the variants have problems to model G_{dh} . SM+MO is the best option but SM+ME and SM+AE are very close. What leads to infer that the errors in this product are not related exclusively to the atmospheric inputs, but are probably a product of the other options selected as fixed in the model, or are due to limitations of the model to reproduce diffuse irradiance accurately. For instance, the parametrizations in the reference atmosphere or the aerosol model do not adjust enough to the characteristics of this case. However, as stated previously, being a clear-sky model, the diffuse component is but a small part of global irradiance (of the order of 12 to 20 %) so this has limited impact on global accuracy.

Finally, G_h is a product calculated from closure equation, thus it includes any errors that G_b and G_{dh} may have. A result that comes as a surprise is the good performance of SM+DE, where a small bias and dispersion are achieved, coming from G_b and G_{dh} that had bad performances. This is explained because of compensation of errors in G_{dh} and G_b . The result of SM+AE for

G_h with default inputs is associated with a large dispersion and a very low bias, resulting from partial cancellation of errors from G_b and G_{dh} . The results for SM+ME and SM+MO close to each other, suggesting both data sources are equally good to estimate G_h .

4.4. Conclusions

SMARTS is a powerful tool to estimate clear-sky spectral and broadband irradiance, in its global, diffuse and direct versions. It is customizable, offering a wide range of possibilities and details to add, to match the user needs, giving performance results that are computationally efficient and with an accuracy which is competitive with that of more sophisticated radiation transfer calculations.

The model has given a good performance when tested broadband against a selection of clear sky samples from a large data set of 5 years. It has also given good results when tested against a small data set of around 100 samples of spectral irradiance.

The atmospheric inputs definitely play an important role in the results of the model performance, having been MODIS-AQUA and MERRA-2 the two data sources that showed a better representation of the atmospheric composition in time. Using the default parameters is not an adequate option when it comes to obtaining good results because they will misrepresent the instantaneous atmospheric conditions and they are also not locally adapted. Similarly, using a distant AERONET station is not recommendable because the spatial variability introduces uncertainties. If the AERONET station is not within 20 km round (Ichoku et al., 2002; Sani et al., 2024), it is preferable to use a reanalysis data base.

The most challenging variable to model accurately was $G_{dh,\lambda}$, showing a positive bias of the order of 20-30 W/m²μm with all the atmospheric inputs tested. That suggests this bias is independent of the atmospheric input and is instead related to the way SMARTS estimates diffuse irradiance. However, under clear-sky conditions, diffuse irradiance is a small part of global irradiance and this is not a mayor limitation in most applications.

On the other hand, the results from using one single spectroradiometer to measure both $G_{h,\lambda}$ and $G_{dh,\lambda}$ and infer $G_{b,\lambda}$ with the measurement scheme proposed worked well, the modelled versus measured comparisons showed it to give good results.

Chapter 5

Assessment of the clear-sky broadband irradiance model REST2

This section is based on the work presented at the Brazilian Congress of Solar Energy (Congresso Brasileiro de Energia Solar, CBENS) 2022, Florianópolis, Brasil: Performance of the REST2 Model for 1-minute Clear-Sky Solar Irradiance with MERRA-2 Atmospheric Inputs. Russo, P., Laguarda, A., Abal, G., Piccioli, I. (2022), available at: doi: <https://doi.org/10.59627/cbens.2022.1100>. In this section, the methodology is updated, using a different sample selection for the validation data set, and changing the constraints on the atmospheric inputs. The performance indicators have been updated accordingly.

Nowadays, several broad-band clear-sky models have been proposed and are in use worldwide. A review of seventy such models can be found in (Antonanzas-Torres et al., 2019). These models require inputs describing the state of the atmosphere and produce broadband global solar irradiance on a horizontal plane and one or both of its components. The simplest models can use one effective input to describe the atmosphere. An example is the ESRA model (Rigollier et al., 2000). This model uses the Linke Turbidity (Linke, 1922), and, if it is locally determined, it can provide hourly horizontal global irradiance with reasonable accuracy (Laguarda and Abal, 2020). More precise models such as SMARTS or McClear (Lefèvre et al., 2013) use several atmospheric inputs and have the potential to achieve good accuracy, provided those inputs are available with the required time scales and with low uncertainty. This is not typically the case at most locations and one must rely on satellite-based estimates for atmospheric parameters such as water vapour or aerosol content.

One of the most detailed clear-sky models in use is REST2 (Gueymard, 2008b), which is based on a parametrization of radiative transfer models and related to the SMARTS spectral model (Gueymard, 2005), discussed in Chapter 4. REST2 is widely used as a sub model for all-sky satellite based models. For instance, it is the clear-sky component of the Physical Solar Model (PSM) (Habte et al., 2017), by NREL and NASA.

REST2 models solar beam irradiance attenuation in two broadband regions: band 1 (ultraviolet

or UV + visible or VIS) at 290 - 700 nm and band 2 (infrared or IR) at 700-4000 nm. In the UV region, attenuation is mainly due to ozone absorption. In the VIS region attenuation is mainly due to Rayleigh scattering by air molecules and scattering and absorption by aerosols. In the IR region, attenuation is mainly due to water vapour and other residual gasses in the atmosphere. The model produces estimates for beam normal irradiance (G_b), global horizontal irradiance (G_h), diffuse horizontal irradiance (G_{dh}), PAR irradiance ($G_{h,PAR}$) and illuminance. It uses up to eight input variables, which are: precipitable water vapour (w , cm), the Ångström turbidity parameters (α_1 , α_2 , β), local atmospheric pressure (p , hPa), ozone column (u_o , cm) and the ground scattering albedos for band 1 and band 2, ρ_{g1} and ρ_{g2} . It allows generic values to be used when the local information is not available. Most relevant among these input variables are precipitable water vapour and the Ångström turbidity parameters describing the aerosol content. These can be obtained (for any site worldwide) from the reanalysis data base MERRA-2 (Gelaro et al., 2017), as discussed in Section 2.4.

In this chapter, the REST2 model is evaluated at 1-min timescale against quality controlled ground data of G_h , G_{dh} , G_b and $G_{h,PAR}$ irradiances, in the site Salto (see Table 2.2 for coordinates). Estimates from MERRA-2 are used to obtain the required atmospheric information. Thus, the validation is for the REST2 model in the region of interest, when used with MERRA-2 inputs.

5.1. Model overview

REST2 is based on SMARTS parametrizations, therefore it inherits a compromise between good performance and computing efficiency. A thorough description of REST2 algorithms can be found in Gueymard (2008b). Here, it is included only a brief summary. As mentioned, the model considers two sub-bands: band 1 covers $290 \text{ nm} \leq \lambda < 700 \text{ nm}$, and band 2 covers $700 \text{ nm} \leq \lambda < 4000 \text{ nm}$. From here on, subindexes $i = 1$ and 2 will be used for referring to each sub-band. The model works separately with each sub-band, and then sums both bands to obtain the broadband irradiance. To begin with, it considers the values of the mean extraterrestrial irradiance at mean Sun-Earth distance is: $G_{0,1} = 635.4 \text{ W/m}^2$ and $G_{0,2} = 709.7 \text{ W/m}^2$ (Gueymard, 1994). These values are obtained by the integration of the TOA reference solar spectrum in the relevant ranges (Gueymard, 1994). Note that the values imply a rather low value of the solar constant of 1345.1 W/m^2 , which is about 1 % below the currently accepted value of 1361 W/m^2 (Kopp and Lean, 2011).

5.1.1. Beam normal irradiance

Broadband $G_{b,i}$ (W/m^2) is calculated as the sum of $G_{b,i}$ (W/m^2) (Eq. 5.1), being $i = 1$ and 2 the notation for each band. $G_{b,i}$ is by definition the integral of $G_{b,\lambda}$ (see Eq. 2.3 for details).

$$G_b = G_{b,1} + G_{b,2}. \quad (5.1)$$

$G_{b,i}$, is obtained as a product of the average effective transmittances (T'_i) corresponding to the atmospheric components considered (noted as subindexes described in Table 4.1).

$$G_{b,i} = G_{0,i} T'_{ri} T'_{gi} T'_{oi} T'_{ni} T'_{wi} T'_{ai}. \quad (5.2)$$

T'_i are multiplied since it is assumed their effects are independent from each other. In the same way as in Eq. (4.1), these transmittances are assumed to be independent so their product is the total transmittance. Each T'_i has a parametric expression obtained from running SMARTS (version 2.9.5) varying the inputs, and fitting the transmittance results of SMARTS against the sensitive parameter related to that transmittance, using a determined parametric polynomial expression. These expressions will not be detailed in here, but are available in Gueymard (2008b). For each process an individual optical air mass is considered: m_R , m_o , m_w , m_a (Section 2.2 and Appendix B.3 show their detailed expressions). To calculate T'_i , the model requires: site pressure (p , hPa), ozone column (u_o , cm), nitrogen dioxide column (u_n , cm), precipitable water vapour (w , cm), Ångström parameters (α_i and β_i , unitless). The corresponding constraints of these coefficients are shown in Eq. (5.3),

$$\beta_1 = \beta \cdot 0.7^{\alpha_1 - \alpha_2}, \quad \beta_2 = \beta. \quad (5.3)$$

When it is not possible to determine α_i and β_i , it can be assumed that $\alpha_i = \alpha$.

The aerosol transmittance is calculated as Eq. (5.4), using Eq. (2.23)

$$\tau_{ai} = \beta_i \lambda_{ei}^{-\alpha_i}, \quad T_{ai} = e^{-m_a \tau_{ai}}, \quad (5.4)$$

where: λ_{ei} are the effective wavelengths for each band (calculated as a function of the aerosols air mass and the coefficient β).

The aerosol scattering transmittance for each band, T_{asi} , is calculated from Eq. (5.5),

$$T_{asi} = e^{-m_a \omega_{gi} \tau_{ai}}, \quad (5.5)$$

where: ω_{gi} are the single scattering albedos for each band. Their typical values are: $\omega_{g1} = 0.92$ and $\omega_{g2} = 0.84$ respectively, see Appendices B.6 and B.7 for details.

5.1.2. Diffuse and global horizontal irradiance

The diffuse irradiance is modelled using two layers in the atmosphere: one on the top and one on the bottom. In the top layer it is assumed that the relevant processes are Rayleigh scattering, ozone and mixed gases absorption, while in the bottom layer the processes are aerosol scattering and absorption, water vapour and nitrogen dioxide scattering. When the irradiance reaches the top layer, Rayleigh scattering takes place, it is supposed then that the diffuse irradiance that continues downwards behaves as beam irradiance at an effective fixed air mass of $m' = 1.66$ (corresponding to an effective zenith angle of about 53 degrees), which is used for the calculus

of all the transmittances related to absorption processes. The incident diffuse irradiance ($G_{dhp,i}$) on a perfectly absorbing horizontal surface (with albedo equal to zero) is parametrized as:

$$G_{dhp,i} = G_{0,i} \cos \theta_z T'_{oi} T'_{gi} T'_{ni} T'_{wi} [B_{Ri}(1 - T_{Ri}) T_{ai}^{0.25} + B_a F_i T_{Ri} (1 - T_{asi}^{0.25})], \quad (5.6)$$

where: F_1 and F_2 are correction factors that serve to compensate the error introduced by the simplified transmittance approach. B_a is the aerosol forward scatter factor. B_{Ri} are the forward scattering fractions for Rayleigh extinction (if there was no multiple scattering, their value would be 0.5 (assuming that half the scattered irradiance is reflected to space). This is the case of sub-band 2 (IR), where multiple scattering is considered negligible, and $B_{R2} = 0.5$). B_{R1} is a broadband ratio representing the direct to global irradiance relationship. It is calculated applying the empirical parametrization from (Skartveit and Olseth, 1988):

$$B_{R1} = 0.5 (0.89013 - 0.0049558 m_R + 0.000045721 m_R^2). \quad (5.7)$$

Finally, B_a , represents the fraction of aerosol scattered radiation directed in the forward (solar) direction. It accounts for the anisotropy of aerosol scattering and affects the amount of diffuse irradiance reaching the surface. It is calculated as:

$$B_a = 1 - e^{-0.6931 - 1.8326 \cos \theta_z}. \quad (5.8)$$

For an ideal black surface, the beam incident irradiance would be $G_{bp} = G_{b,1} + G_{b,2}$, and the diffuse and global (G_{dhp} , G_{hp}) would be:

$$\begin{aligned} G_{dhp} &= G_{dhp,1} + G_{dhp,2}, \\ G_{hp} &= G_{bp} \cos \theta_z + G_{dhp}. \end{aligned} \quad (5.9)$$

The ground albedo, ρ_g corresponds to the average albedo of a large area of 5-50 km around the site. The sky albedo is obtained separately for each band as a function of α_i and β_i . Using it, the back scattered diffuse components, $G_{dhd,i}$, are obtained considering multiple reflections between the ground and the atmosphere, as shown in Eq. (5.10),

$$G_{dhd,i} = \rho_{gi} \rho_{si} (G_{b,i} \cos \theta_z + G_{dhp,i}) / (1 - \rho_{gi} \rho_{si}). \quad (5.10)$$

Notice $G_{dhd,i}$ has the same structure as Eq. (4.17) from SMARTS, which also includes the effects of multiple reflections and results from the summation of an infinite series, or backscattering.

Following, the total diffuse irradiance is calculated separately for each band as the sum of the diffuse in a perfectly absorbing surface plus the diffuse backscattered:

$$G_{dh,i} = G_{dhp,i} + G_{dhd,i} \quad (5.11)$$

Afterwards, the broadband diffuse irradiance is calculated as:

$$G_{dh} = G_{dh,1} + G_{dh,2} \quad (5.12)$$

Finally the broadband global horizontal irradiance is calculated with closure (Eq. 2.6).

5.1.3. Previous validations for REST2

Several validations of G_h , G_{dh} and G_b from the REST2 model have been done in different parts of the world. The sites studied are mainly located in Europe, North America, North Africa, the Middle East, and more rarely, in the Southern Hemisphere or South America, at 1-minute frequency. The validations carried out by Gueymard (2012), Engerer and Mills (2015) and Antonanzas-Torres et al. (2019) stand out, because they are recent, for temperate climates (such as the region of interest in this work), and because the three products of irradiance are considered (except for Engerer and Mills (2015), which omits G_{dh}). Table 5.1 shows the average results from these studies in terms of rMBD and rRMSD.

Table 5.1: Performance metrics for REST2 estimates at 1-minute level on previous validations worldwide. rMBD and rRMSD are expressed as % of the average of the measurements. To convert into absolute values, only (Gueymard, 2012) provides the mean observed values, which are in average: $G_h = 675.6 \text{ W/m}^2$, $G_{dh} = 97.3 \text{ W/m}^2$ and $G_b = 856.8 \text{ W/m}^2$.

Study/variable Metric	G_h		G_{dh}		G_b	
	rMBD	rRMSD	rMBD	rRMSD	rMBD	rRMSD
Gueymard, 2012	-0.2	1.5	-0.4	8.8	-0.3	1.4
Engerer and Mills, 2015	+0.4	5.1	—	—	-0.3	4.7
Antonanzas et al., 2019	-0.4	3.1	-1.0	5.8	-0.3	7.9

These works compare a large number of clear-sky models and all of them rank REST2 between those with the highest performances. Gueymard (2012) validates REST2 estimates with AERONET atmospheric information over 4 measurement's sites in the USA and one in Saudi Arabia. The validation, on a scale of 1-3 minutes, concludes that good models can estimate G_h with precision close to that of measurement instruments, being the G_b the most complex to model due to its strong dependence on aerosols contents. Engerer and Mills (2015) carry out a validation study of 9 models at 14 sites in Australia on a minute scale using interpolated atmospheric mean values extracted from the SoDa dataset (Rigollier et al., 2001). Antonanzas-Torres et al. (2019) carried out an extensive validation of 70 clear sky models at two BSRN stations in Europe at the 1-minute level. The aerosol optical depth and water vapor content information is obtained from local AERONET measurements. The results in Table 5.1 show that when the model is used with good quality atmospheric in-situ information it can provide high accuracy, similar to the accuracy of the measurement instruments.

In the region of interest of this work, previous validations have been performed, as shown in Table 5.2. Porfirio and Ceballos (2013) performed a validation of G_b from REST2 (among other models) in three sites in northeastern Brazil (Petroлина, Natal and São Luis) using atmospheric inputs from the MODIS and OMI instruments from NASA. On average, the rMBD was +1.6 % and rRMSD was 3.2 %. Laguarda (2021) validated the model at the hourly scale in Salto, Uruguay (among other sites), using MERRA-2 atmospheric information for the period 2015-2017.

For G_h , the model estimates showed an rMBD of -0.9 % and an rRMSD of 3.6 %, while for G_b the rMBD was -4.9 % and the rRMSD was 7.2 %. Subsequently, the present work (Russo et al., 2022) validated the model in Salto, Uruguay, over a longer time span (2017-2020) and for all four broadband outputs (G_h , G_{dh} , G_b , and $G_{h,PAR}$). These results are discussed in the next section. Very limited information was found regarding PAR validation, making it impossible to report rMBD and rRMSD values for temperate sites. To the best of our knowledge, G_{dh} or $G_{h,PAR}$ estimates from REST2 have not been validated in the region of interest.

Table 5.2: Performance metrics for REST2 estimates on previous regional validations. rMBD and rRMSD are expressed as % of the average of the measurements.

Study / Variable Metric	G_h		G_{dh}		G_b		$G_{h,PAR}$	
	rMBD	rRMSD	rMBD	rRMSD	rMBD	rRMSD	rMBD	rRMSD
Porfirio & Ceballos, 2013	–	–	–	–	1.6	3.2	–	–
Laguarda, 2021	-0.9	3.6	–	–	-4.9	7.2	–	–
Russo et al., 2022 (this work)	-1.2	3.2	46.2	53.0	-4.6	7.2	1.1	4.8

5.2. Data and methods

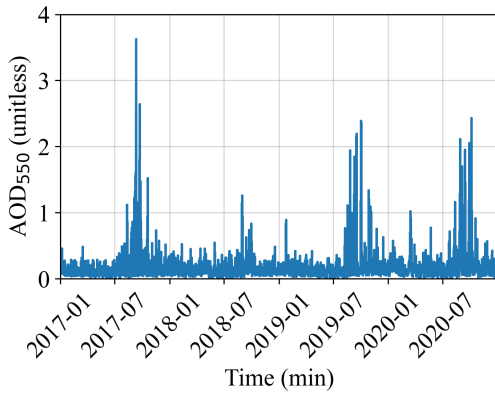
5.2.1. Ground measurements of solar irradiance

Ground measurements of G_h , G_{dh} and G_b were collected in Salto (see Section 2.4). The measurements in this case have been recorded at 1 minute frequency, for a 4 years period from 2017-2020, registering a wide range of climatic conditions. $G_{h,PAR}$ was measured (in $\mu\text{mol}/\text{m}^2\text{s}$) with a Kipp & Zonen PQS1 quantum sensor. $G_{h,PAR}$ is converted from photon flux units ($\mu\text{mol}/\text{m}^2\text{s}$) to irradiance units (W/m^2) using the approximate equivalence $1 \mu\text{mol}/\text{m}^2\text{s} = 0.21964 \text{ W}/\text{m}^2$ (DiLaccio et al., 2024) obtained from the extraterrestrial standard solar irradiance spectrum (Wehrli, 1985), using the methodology described in Appendix B.14. It is important to note this method considers the same irradiance intensity that reaches TOA also reaches the ground surface, which is not true due to spectrally selective atmospheric scattering and absorption.

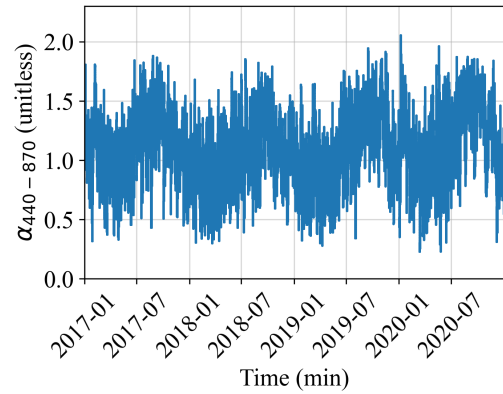
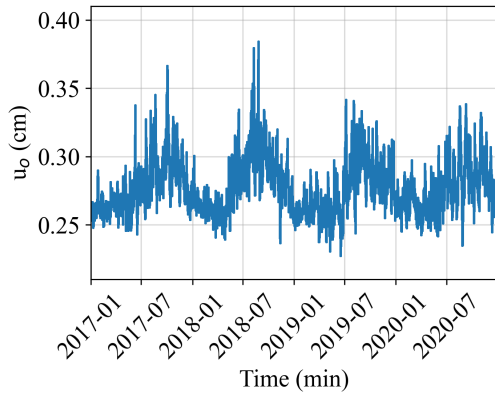
5.2.2. Atmospheric information

The source of atmospheric information is the re-analysis database MERRA-2. The relevant variables used from this database are: Aerosol Optical Depth at 550 nm (AOD_{550} , unitless), Ångström exponent at 440-870 nm (α , unitless), total ozone column (u_o , in Dobson Units or DU) and precipitable water vapour (w , kg/m^2). All variables are downloaded at 1-hour intervals for a box of 0.5×0.625 degrees centred in the latitude and longitude of Salto measurement station for the period of work (2017-2020). In a post-processing step, these variables are linearly interpolated to 1-minute frequency. The original units are converted to the units that REST2 requires as input:

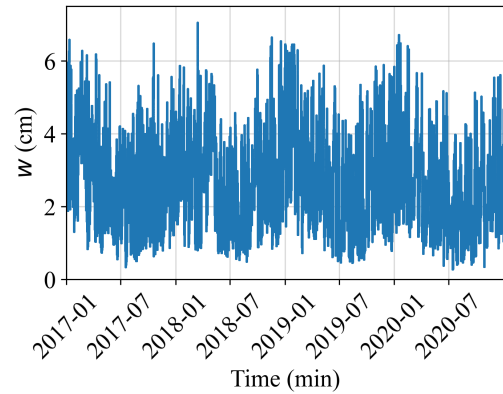
w (cm) = w (kg/m²) $\times$ 0.10 (cm $\cdot$ m²/kg) and u_o (cm) = u_o (DU) $\times$ 0.001 (cm $\cdot$ DU⁻¹). The Ångström Coefficients (β_i , unitless) are calculated using Eq. (5.3). After visual inspection, see Fig. 5.1, it is observed that no filters need to be applied to the variables, and that the fluctuations observed respond to seasonal variations. Altitude was set to 56 masl and atmospheric pressure was set to 1013.25 hPa. Other secondary variables are set to default constant values. The superficial ultraviolet albedo (ρ_{g1} , unitless) and superficial infrared albedo (ρ_{g2} , unitless) are set to a constant value of 0.2, a default value for grasslands according to Gueymard (2005). u_n (cm) is set to a constant value of 0.0002 (equivalent to 200 ppm), as recommended by (Gueymard, 2008b), in the absence of measurements.



(a) Aerosol Optical Depth at 550 nm.

(b) Aerosol Ångström exponent, $\alpha_{440-870}$.

(c) Total columnar ozone.



(d) Precipitable water vapour.

Figure 5.1: Atmospheric variables interpolated to 1 minute frequency, for the period considered, 2017-2020. Figure by Paola Russo.

5.2.3. Quality control and clear-sky selection

The quality control applied over the ground measurements follows the procedure proposed by (Perez-Astudillo et al., 2018) with coefficients adapted to the site LE, as described by (Piccioli, 2022), in page 46, Table 3.3. It includes a set of 19 filters, among them, the Baseline Solar Radiation Network (BSRN) quality control recommendations (McArthur, 2005), and visual inspection, to detect, for example, tracker mis-alignment conditions. Additionally, two filters were applied: a minimum solar altitude, $\alpha_{min} = 7^\circ$, in order to minimize the directional (cosine) errors that affect pyranometers mainly at low solar altitudes, and a PAR filter, to satisfy the following upper and lower bounds, based on (Opálková et al., 2018):

$$0.35 G_{0h,PAR} < G_{h,PAR} < (G_{0h,PAR} - 51.615) \text{ (W/m}^2\text{)}. \quad (5.13)$$

There, $G_{0h,PAR}$ is the solar irradiance on a horizontal plane at TOA (400-700 nm).¹ A summary of the quality control results for each variable (G_h , G_{dh} , G_b , $G_{h,PAR}$) is shown in Table 5.3, where an important portion of the discarded data is related to the solar altitude filter. The data records that passed the quality control are shown in Fig. 5.2 as blue dots.

Table 5.3: Quality control and clear-sky detection results for each variable. The first row shows the number of valid data points. The second row indicates the number of data flagged by quality control (QC), also expressed as a percentage of the valid data. The third row presents the number of clear-sky samples selected, with percentages also relative to the valid data (first row).

variable	G_h	G_{dh}	G_b	$G_{h,PAR}$
diurnal, non-null	1005940	1002159	993599	1042128
pass filters	684756	684729	684756	864762
	(68.1 %)	(68.3 %)	(68.9 %)	(83.0 %)
clear-sky samples	233539	233539	233539	242844
	(23.2 %)	(23.3 %)	(23.5 %)	(23.3 %)

Quality measurements under clear sky conditions are necessary for performing a REST2 validation. This data was selected from the G_h time series using the method proposed by Reno and Hansen (2016), available at the Python library PVlib (detect_clearsky), the clear-sky model used by this method is not determinant since it is adjusted by iteration to the data sample. For this purpose, the ESRA model (Rigollier et al., 2000) was used, assuming an average atmosphere with a fixed $TL = 2.5$. Additionally, data points with high f_d (Eq. 2.7), typically associated with cloudy conditions, were excluded using the two additional filters shown in Eq. (5.14) applied

¹Calculated as $G_{0h,PAR} = G_{s,PAR} \cdot \cos(\theta_z) \cdot F_n$, where F_n is the orbital correction factor, z is the solar zenith angle and $G_{s,PAR} = 530 \text{ W/m}^2$ is the solar constant for the 400-700 nm range, obtained from integration of the extraterrestrial standard solar irradiance spectrum (Wehrli, 1985).

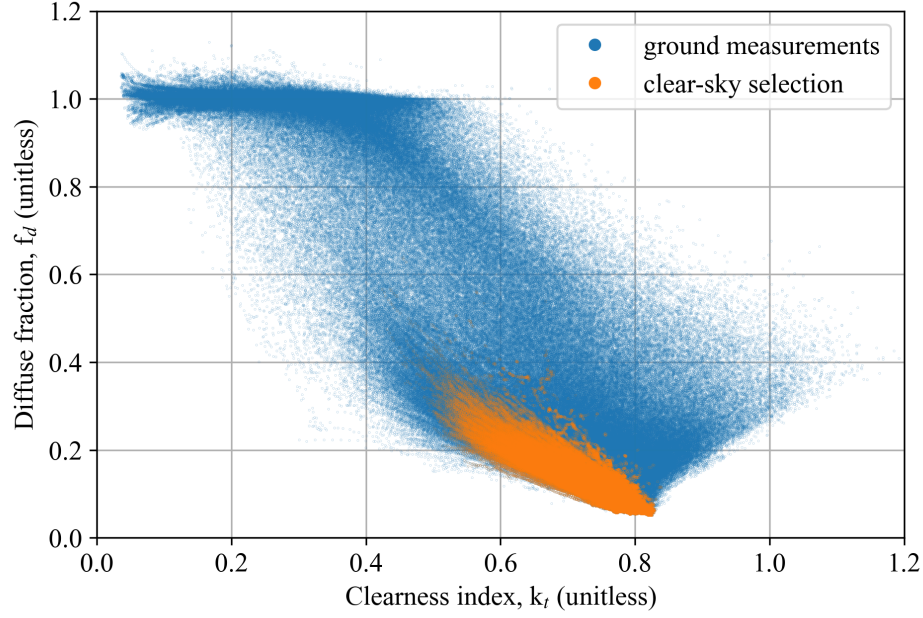


Figure 5.2: Diffuse fraction vs. clearness index (f_d - k_t) diagram, ground quality checked measurements (blue dots) and clear-sky selection (orange dots). Figure by Paola Russo.

to the preliminary clear sky data set (Perez-Astudillo et al., 2018). This filters represent a trapezoidal region in Fig. 5.2, where the clear sky data is located. For details on k_t definition see Eq. (2.8).

$$f_d < 0.6 \quad \& \quad f_d < 1 - k_t. \quad (5.14)$$

The number of clear-sky measurements selected by this procedure is shown in the last row of Table 5.3. The final set of 1-min clear-sky data is shown (orange dots) in the dimensionless diagram (f_d - k_t) presented in Fig. 5.2. The selected clear-sky minute data will be used for the validation.

5.3. Performance of REST2 model

Performance metrics of the assessment of REST2 with LES data and atmospheric inputs from MERRA-2 are presented in Table 5.4. G_h estimates show strong agreement with the measurements, resulting in a small underestimation (rMBD = -1.2 %) and a small dispersion (rRMSD = 3.2 %), close to the typical uncertainty of a pyranometer’s measurement (see Sec. 2.4). The performance of the $G_{h,PAR}$ estimates is similar to G_h , but with a slightly positive bias. In both cases R^2 is very high (greater than 0.99). The model exhibits greater values of relative bias and dispersion for G_{dh} (approximately 46.2 and 53.0 % respectively). Although in absolute terms the RMSD is 36.6 %, smaller than G_b but higher than for $G_{h,PAR}$ and G_h (RMSD around 14 W/m² and 20 W/m² respectively). The low mean of clear-sky G_{dh} accounts for the high values in relative terms. In addition, the estimate-measurement correlation for G_{dh} is weaker, with a value around 0.8. In the case of G_b , the model also underestimates by rMBD = -4.6 %, or in absolute terms -40.1 W/m², and its dispersion is of 4.8 % of the mean. However, this variable presents a better correlation. These results are illustrated in the scatter plots of Fig. 5.3. Greater dispersion is evident in G_b and G_{dh} estimates. Even though the model shows uncertainty in reproducing G_{dh} , under clear sky conditions, G_{dh} typically represents only 10-15 % of G_h .

The current validation using MERRA-2 presents similar biases when compared to the worldwide validations presented in Table 5.1, which use AERONET measurements as atmospheric inputs, which suggests this atmospheric input is appropriate for using in the region. Additionally, at regional scale (as shown in Table 5.2), the biases and dispersions are similar, supporting the results. Particularly, (Laguarda, 2021) also saw a negative bias in G_h and G_b . The underestimation of G_b , may be due to a lower accuracy of the MERRA-2 reanalysis data set over the region of interest. The regional validation of this database (see Table 2.3) shows significant positive biases in AOD and water vapour. This implies greater atmospheric turbidity, which leads to an underestimation of G_b and an overestimation of G_{dh} , as noted in Laguarda and Abal (2020). These two deviations of opposite sign are attenuated in the estimation of G_h and $G_{h,PAR}$, which is only slightly underestimated.

Table 5.4: Performance metrics for REST2 estimates.

metric/variable	G_h	G_{dh}	G_b	$G_{h,PAR}$
rMBD (%)	-1.2	46.2	-4.6	1.1
rRMSD (%)	3.2	53.0	7.2	4.8
correlation (adim)	0.998	0.821	0.928	0.993
average (W/m ²)	641.3	69.1	862.6	291.9

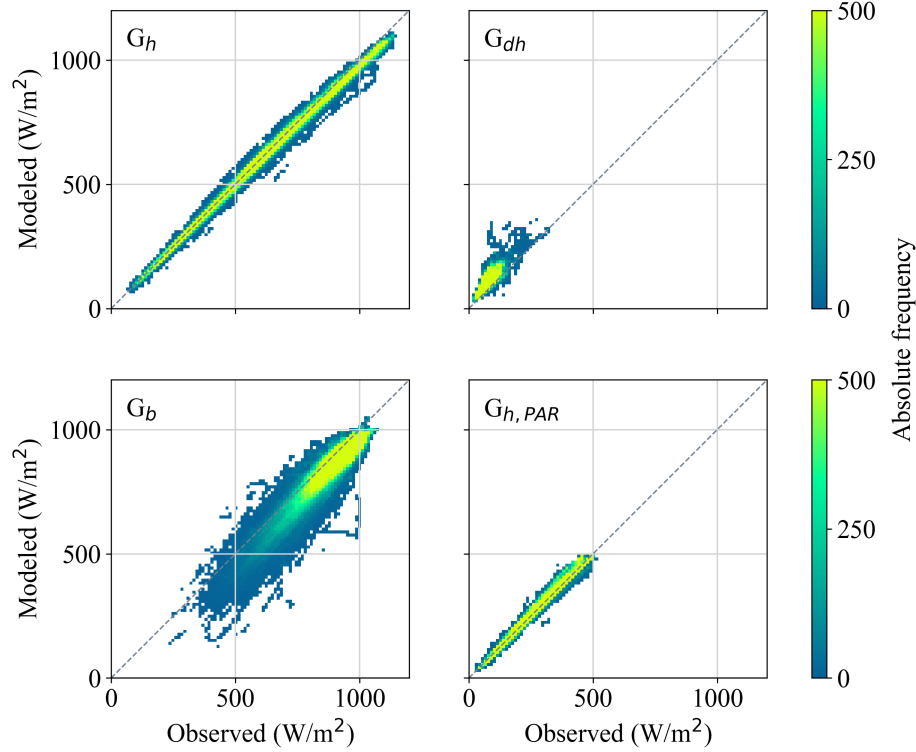


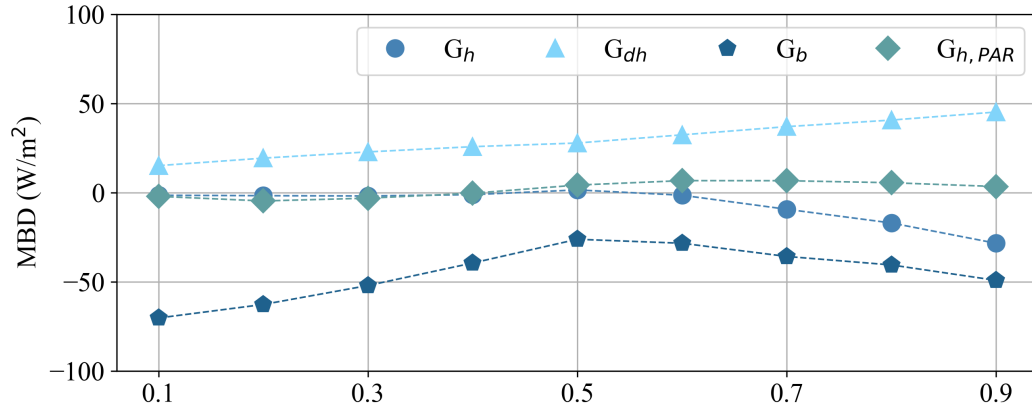
Figure 5.3: Model performance compared to ground measurements for G_h , G_{dh} , G_b and $G_{h,PAR}$. Figure by Paola Russo.

Dependence with solar zenith angle

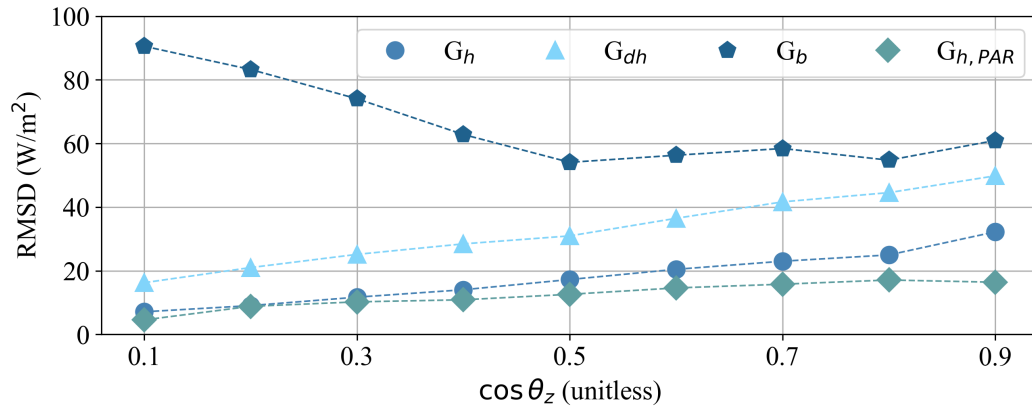
To study the error in terms of solar altitude, the dependence of MBD and RMSD with $\cos \theta_z$ is analyzed. Higher $\cos \theta_z$ values are associated with solar noon, while lower values are associated with low solar altitudes and high relative air mass. Figure 5.4 (a) shows that the model systematically overestimates G_{dh} for all solar altitudes, being the effect more marked for $\cos \theta_z$ greater than 0.5. On the other hand, G_b is underestimated for all values of $\cos \theta_z$, but specially for $\cos \theta_z$ lower than 0.5 (low sun). As expected, these deviations of opposite sign partially cancel in the estimation of G_h , which shows small negative bias increasing towards solar noon. $G_{h,PAR}$ shows the lowest bias and it is stable for all solar altitudes.

Figure 5.4 (b) shows the dependence of the RMSD with $\cos \theta_z$. For G_{dh} , G_h and $G_{h,PAR}$, the

dispersion grows gradually with $\cos \theta_z$. The accuracy of G_b estimates show a marked dependence on $\cos \theta_z$. The dispersion is high at low $\cos \theta_z$ (higher air mass) and it stabilizes at a low value for $\cos \theta_z$ greater than 0.5 (low air mass). This reflects the fact that REST-2 models G_b using a product of atmospheric transmittances, an approximation which is less accurate at high air masses.



(a)



(b)

Figure 5.4: Model performance for G_h , G_{dh} , G_b and $G_{h,PAR}$ for different $\cos \theta_z$. Figure by Paola Russo.

5.4. Conclusions

The REST2 clear-sky model with atmospheric inputs (precipitable water vapour, AOD_{550} and ozone column) from MERRA-2 was evaluated against 1-min data from LES. The evaluation was performed at 1-minute timescale using clear sky measurements automatically selected by an algorithm from 4 years of controlled quality ground data. The validation includes the four irradiance outputs of the model, G_h , G_{dh} , G_b and $G_{h,PAR}$.

Over the region of interest, REST2 used with MERRA-2 inputs can estimate G_h and $G_{h,PAR}$ with a typical uncertainty (in terms of rRMSD) of -1.2 % and 1.1 % of the mean, respectively. G_b can be estimated with a typical uncertainty of -4.6 %. When modelled G_b is used, it should be considered that this variable presents a negative bias, mainly at low solar altitudes (high air mass). G_{dh} , a variable with a secondary role under clear sky conditions, is estimated with an over-estimation of 46.2 % and higher relative uncertainty (53.0 %).

Previous studies suggest that REST2 can be very accurate when used with high quality AOD and w in situ measurements, usually from AERONET sites. This information is not available for most locations, thus it is relevant to assess the model using MERRA-2 reanalysis data, which is available worldwide at 1 hour intervals. In the region of study, the MERRA-2 database tends to overestimate the AOD and w . As noted in previous works, this results in a systematic under-estimation of G_b and an over-estimation of G_{dh} . These effects partially cancel and result in a small underestimation of G_h . On the other hand, the hourly data from MERRA-2 base may represent the intra day variability of the atmosphere, and this makes it potentially useful for capturing intra-day trends in clear-sky solar irradiance, provided a post-processing (local adaptation) is applied to the initial estimates. These improvements in the atmospheric information and also data from the surface albedo (that can affect mainly the G_{dh}) are left for future work. These simple procedures are expected to significantly reduce the bias and improve the overall performance of the REST2 model when used with MERRA-2 inputs.

An additional observation can be made when comparing the results of REST2 with MERRA-2 atmospheric inputs (Table 5.4) the results of SM+ME (Table 4.12). Overall, SM+ME outperformed REST2, specifically, the biases in G_{dh} and G_b , and its dispersions were better, showing a 10 and 2 % reduction respectively, with regard to REST2 performance indicators. Only in G_h , REST2 bias was better than SMARTS, this could be due to error compensation, but still REST2 had worse dispersion. The bias in G_h also changed its sign (in SMARTS it was positive 1.7 % and in REST2 it was negative -1.2 %). The better performance of SMARTS can be explained because it models the transmittance of the atmosphere with more spectral resolution, meaning the spectral irradiance behaviour is represented better, resulting in more accurate broad band estimates. Whereas REST2 models an average transmittance for each of the two sub-bands, and therefore the spectral description is rather simplified, leading to less precise broadband estimates. Since both models calculate the G_h as the sum of the components G_{dh} and G_b , in both cases G_h has a compensated bias, which tends to be low and close to the instrument's uncertainty.

Chapter 6

Retrieval of Aerosol Optical Depth from spectral irradiance ground measurements

This work was presented in ISRSE-39th Symposium, Antalya, Turkey, 24-28th April, 2023. Its full text is published in the International Society of Photogrammetry and Remote Sensing (ISPRS) Archives, and available at: doi: <https://doi.org/10.5194/isprs-archives-XLVIII-M-1-2023-565-2023>, and <https://ui.adsabs.harvard.edu/abs/2023ISPAr48M1..565R/abstract>

As discussed in Chapter 2, AOD_λ (or also denoted as $\tau_{a\lambda}$, for practicality purposes in this chapter) is an important atmospheric parameter because it quantifies the radiative extinction (due to scattering and absorption) caused by aerosol content in a vertical column of the atmosphere, at a specific wavelength (WMO/GAW, 2016). The most common technique used to estimate $\tau_{a\lambda}$ consists of measuring the monochromatic solar beam irradiance, and estimating the attenuation that occurs between the top of the atmosphere (TOA) and the surface level.

Table 6.1: Comparison of retrieved $\tau_{a\lambda}$ from EKO MS-711 measurements against AERONET estimates: García-Cabrera et al. (2020) - GC, Qiao et al. (2023) - Q. Performance is evaluated with the mean bias deviation (MBD, unitless) and the root mean squared deviation (RMSD, unitless), relative to the reference mean values.

λ (nm)	MBD		RMSD	
	GC	Q	GC	Q
340	0.007	na	<0.001	na
380	0.005	0.003	<0.001	0.026
440	0.005	-0.011	0.001	0.024
500	0.005	<0.001	0.002	0.020
675	0.006	0.009	<0.001	0.021
870	0.003	-0.012	<0.001	0.020

In this chapter, the results of retrieving aerosol optical depth, $\tau_{a\lambda}$, at six wavelengths (340, 380, 440, 500, 675, 870 nm) will be presented. Notice throughout the chapter, the retrieval will be denoted as $\tau_{a\lambda}$ to differentiate it from the reference value from AERONET, which will be denoted $\tau_{a\lambda}^0$, both are wavelength dependent.

As reference, results of recent studies are included in (García-Cabrera et al., 2020; Gröbner and Kouremeti, 2019; Qiao et al., 2023), where they have used measurements from an EKO MS-711 collimated spectroradiometer measurements to retrieve $\tau_{a\lambda}$ at multiple wavelengths, obtaining the results shown in Table 6.1.

6.1. Methodology

The methodology used is schematized in Figure 6.1. Firstly, ground measurements of $G_{b,\lambda}$ are taken with a collimated spectroradiometer (EKO MS-711, Section 2.4) at Montevideo (Table 2.2). Then, wavelengths are selected in order to compare the results with AERONET's database retrievals. Following, the inversion algorithm is applied, combining the Lambert-Beer-Bouguer Law (Eq. 2.20) with the Langley Plot Method (Giles et al., 2019; Holben et al., 1998). This approach implies understanding the attenuation processes involved in the atmosphere, such as Rayleigh scattering and gas absorption. Finally, the accuracy of $\tau_{a\lambda}$ is evaluated by comparison with simultaneous AERONET reference data, $\tau_{a\lambda}^0$.

AERONET data is routinely registered, and its deduced from CIMEL sun photometer observations. The period considered is during spring in the southern hemisphere, from September to November, 2022. Figure 6.2 shows the spectral irradiance measured at one instant and the vertical lines (green) indicate the wavelengths for the retrieval.

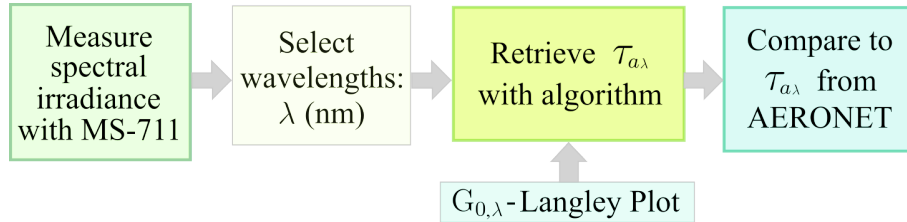


Figure 6.1: Methodology scheme. Figure by Paola Russo.

To apply the inversion algorithm, each irradiance measurement must simultaneously comply with the following requirements:

- i) correspond to clear-sky and stable atmospheric conditions, passing strict visual inspection to discard instants that could correspond to unstable atmospheric conditions, cirrus clouds, erroneous measurements.

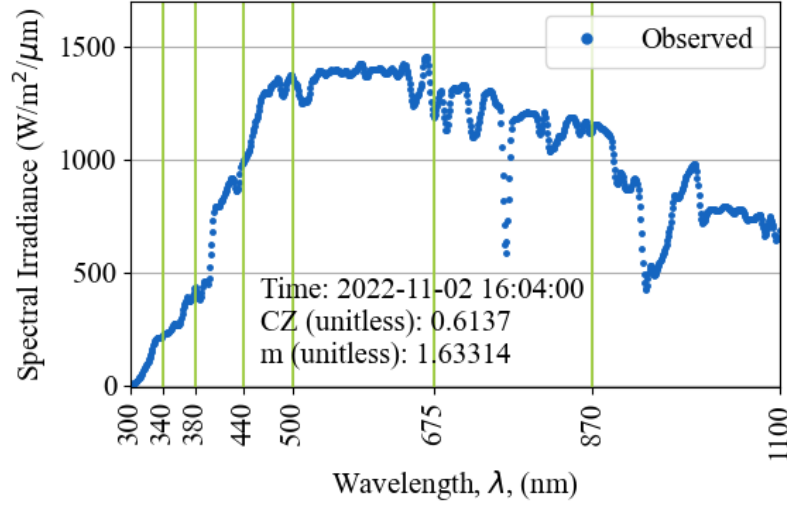


Figure 6.2: Example of measured spectral irradiance. Measurements taken at Montevideo. Figure by Paola Russo.

- ii) Have a simultaneous AERONET measurement available.

AERONET measurements correspond to the 1.5 quality level, which includes a clear-sky selection (Holben et al., 1998). That selection is double checked here with an automated clear-sky selection algorithm based on Reno and Hansen (2016) criteria, using the auxiliary G_h measurements, plus visual inspection on the integral of $G_{b,\lambda}$ measured, in $\lambda = 300$ to 1100 nm (which is $G_{b,EKO}$). Once the preliminary $\tau_{a\lambda}$ is retrieved for every wavelength and every instant, a manual post processing stage is applied, to discard anomalous values coincident with suspiciously unstable sky conditions according to $G_{b,EKO}$. The final selection consists of 2629 instants from 46 different days, in the selected spring period. These are distributed during morning (26 %), noon (29 %) and afternoon (45 %). As an example, the G_h and $G_{b,EKO}$ are shown in Fig. 6.3 for two of these days.

6.1.1. Inversion Algorithm

The law of exponential attenuation (Lambert-Beer-Bouguer) (Eq. 2.20) states that:

$$G_{b,\lambda} = G_{0,\lambda} e^{-\tau_{\lambda} m} \quad (6.1)$$

where, $G_{b,\lambda}$ is the beam normal spectral irradiance at ground level, $G_{0,\lambda}$ is the beam normal spectral irradiance at TOA, computed as $G_{0,\lambda} = G_{s,\lambda} \times F_n$, being $G_{s,\lambda}$ the TOA solar spectral

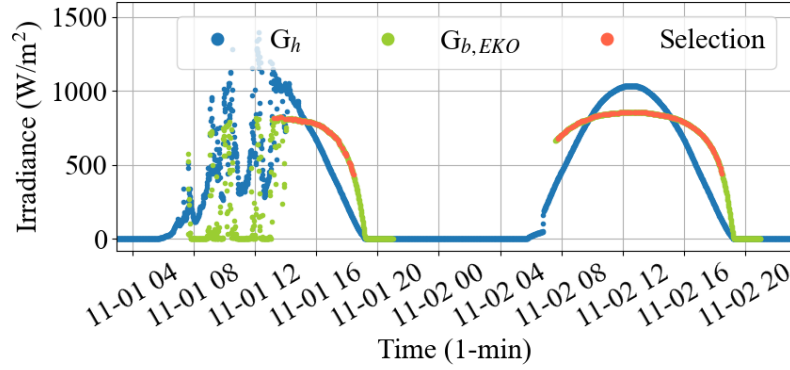


Figure 6.3: Selection of clear-sky instants for two sample days (November 1 and 2, 2022). The x-axis shows the time labels in local time (UTC-3). Figure by Paola Russo.

irradiance estimated using the Langley Plot Method (described in Section 6.1.3). In Eq. (6.1), m is the relative air mass (Eq. 2.12) and τ_λ is the total optical depth.

The contributions to the attenuation of the solar beam considered are: Rayleigh scattering (r), aerosols (a), water vapour (w), and absorption by atmospheric gases: NO_2 (n) and O_3 (o). Assuming their effects are independent from each other, $\tau_\lambda m$ can be expressed as:

$$\tau_\lambda m = \tau_{r\lambda} m_R + \tau_{a\lambda} m_a + \tau_{w\lambda} m_w + \tau_{n\lambda} m_n + \tau_{o\lambda} m_o \quad (6.2)$$

The relevant absorptions for the selected wavelengths are described in Table 6.2. Note that, for these particular wavelengths, water vapour plays a negligible role (Giles et al., 2019).

Table 6.2: Relevant optical depths considered in Eq. (6.1), for each wavelength of study.

Wavelength, nm	Optical depths
340	$\tau_{r\lambda}, \tau_{n\lambda}, \tau_{o\lambda}$
380	$\tau_{r\lambda}, \tau_{n\lambda}$
440	$\tau_{r\lambda}, \tau_{n\lambda}$
500	$\tau_{r\lambda}, \tau_{n\lambda}, \tau_{o\lambda}$
675	$\tau_{r\lambda}, \tau_{o\lambda}$
870	$\tau_{r\lambda}$

The relative air masses corresponding to these processes are calculated as follows. The inverse air mass related to Rayleigh scattering is (Kasten, 1996)

$$m_R^{-1} = \cos \theta_z + 0.50575 \times (96.07995 - \theta_{zd})^{1.6364}, \quad (6.3)$$

where θ_z is the solar zenith angle (radians) and θ_{zd} is its expression in degrees. The inverse air mass related to the NO₂ optical depth (Gueymard, 1995) is

$$m_n^{-1} = \cos \theta_z + 602.30 \times \theta_{zd}^{0.5} (117.960 - \theta_{zd})^{-3.4536}. \quad (6.4)$$

The inverse air mass related to aerosols (Kasten, 1964) is

$$m_a^{-1} = \cos \theta_z + 0.1500 \times (93.885 - \theta_{zd})^{-1.253} \quad (6.5)$$

and the air mass related to Ozone (Komhyr and Grass, 1989) is

$$m_o = \left[1 - \left(\frac{R + h_s}{R + h} \right)^2 \sin^2 \theta_z \right]^{-1/2} \quad (6.6)$$

where $R = 6371.229$ km is the mean radius of the Earth, $h = 22$ km is the mean height of the stratospheric ozone layer and h_s is the station height above mean sea level, in this case $h_s = 0.058$ km.

Rayleigh optical depth is calculated as shown in Eq. (6.7) (Hansen and Travis, 1974), where $p_0 = 101.325$ kPa is the atmospheric pressure at sea level and p is the measured atmospheric pressure in kPa at the site and λ the wavelength in μm .

$$\tau_{r\lambda} = \frac{p}{p_0} \cdot \frac{0.008569}{\lambda^4} \times \left(1 + \frac{0.0113}{\lambda^2} + \frac{0.00013}{\lambda^4} \right) \quad (6.7)$$

The Nitrogen Dioxide optical depth is the product of its column density and its absorption cross section,

$$\tau_{n\lambda} = u_n \cdot \sigma_n(\lambda) \quad (6.8)$$

where u_n (molecules/cm²) is the nitrogen dioxide column obtained from AERONET and $\sigma_n(\lambda)$ (cm²/molecules) is the absorption cross section for NO₂ obtained from HITRAN (Rothman et al., 1992), as the average cross section obtained from the cross sections corresponding to atmospheric temperatures of 220 K and 294 K. Similarly, the optical depth for ozone is

$$\tau_{o\lambda} = u_o \cdot \sigma_o(\lambda) \quad (6.9)$$

where the total ozone column (u_o , cm²/molecules) is given by AERONET. The absorption cross section for O₃, $\sigma_o(\lambda)$ (cm²/molecules), for $\lambda = 340$ nm is obtained from HITRAN, using the average cross section obtained from the cross sections corresponding to five atmospheric temperatures (193, 213, 253, 273, 293 Kelvin) and for $\lambda = 500$ and 675 nm, it is as given in (Burrows et al., 1999).

Finally, the aerosol optical depths, $\tau_{a\lambda}$, are obtained from combining Eqs. (6.1) and (6.2).

$$\tau_{a\lambda} = \frac{1}{m_a} \left[\ln \left(\frac{G_{0,\lambda}}{G_{b,\lambda}} \right) - \tau_\lambda m \right], \quad (6.10)$$

where m is the relative optical air mass, explained in Young (1994) approximation, Eq. (2.11), and τ_λ is the total spectral optical depth, explained in Eq. (2.15).

6.1.2. Circumsolar Correction

The EKO spectroradiometer has a Field of View (FOV) of 5° , and the CIMEL sun photometer has a FOV of 1.2° . The FOV recommended by WMO for AOD retrievals is less or equal to 2.5° (WMO/GAW, 2004). Thus, a larger portion of circumsolar radiation is counted as $G_{b,\lambda}$ by the EKO instrument. For this reason, a circumsolar correction needs to be applied to minimize this effect. It consists of subtracting from the measured direct normal spectral irradiance, $G_{b,\lambda}^{obs}$ ($\text{W/m}^2\mu\text{m}$), an estimation of the circumsolar portion, to obtain an estimate of the spectral irradiance that comes from within 1.2° of the Sun-Earth direction. For this, the circumsolar ratio (CR) is used. It is the fraction of the raw observed spectral irradiance that is circumsolar, thus, the corrected spectral irradiance is

$$G_{b,\lambda} = G_{b,\lambda}^{obs}(1 - CR). \quad (6.11)$$

CR depends on the FOV of the instrument, the wavelength and the $\tau_{a\lambda}$ during a particular instant. For the EKO MS-711 instrument, CR has previously been modelled with the radiative transfer code MODTRAN[®] by García-Cabrera et al. (2020). The resulting CR values as a function of $\tau_{a\lambda}$, are shown in Figure 6.4 and adapted from García-Cabrera et al. (2020), and are used here as a lookup table. For example, for high aerosol loads and low wavelengths, CR may be of 0.05, as shown in Fig. 6.4, in that case 5 % of the measured spectral irradiance is circumsolar. The procedure for correcting the measurement, consists of estimating CR from the curves of Fig. 6.4, using a $\tau_{a\lambda}$ obtained from the preliminary measurement of $G_{b,\lambda}^{obs}$. Then, the measurement is corrected by extracting the estimated circumsolar contribution, using Eq. (6.11). The procedure to calculate $\tau_{a\lambda}$ is an iterative process where an initial $\tau_{a\lambda}$ must be proposed as a seed.

6.1.3. TOA Spectral Irradiance

The solar spectral irradiance that the instrument would have measured if it was at TOA, $G_{s,\lambda}$, is estimated applying the Langley Plot method (Holben et al., 1998; Langley, 1881). This method uses Eq. (6.1) to obtain

$$\ln \left(\frac{G_{b,\lambda}}{F_n} \right) = \ln(G_{s,\lambda}) - \tau_\lambda m \quad (6.12)$$

Assuming a nearly constant total optical depth, τ_λ , Eq. (6.12) implies a linear dependence between the logarithm of the spectral irradiance and the air mass. With a linear coefficient $a = -\tau_\lambda$, and an independent term $b = \ln(G_{s,\lambda})$. This method requires stable atmospheric conditions for its validity, so it must be applied over short periods of time and under clear-sky conditions. Within such stable period, N measurements are taken, to which a least squares regression is performed providing the optimal values for a and b . Finally, $G_{s,\lambda} = e^b$. This procedure is commonly called the calibration of the instrument, even though it is a pseudo-calibration. It is best to have very low $\tau_{a\lambda}^0$ during the instants selected to calibrate the instrument, for example,

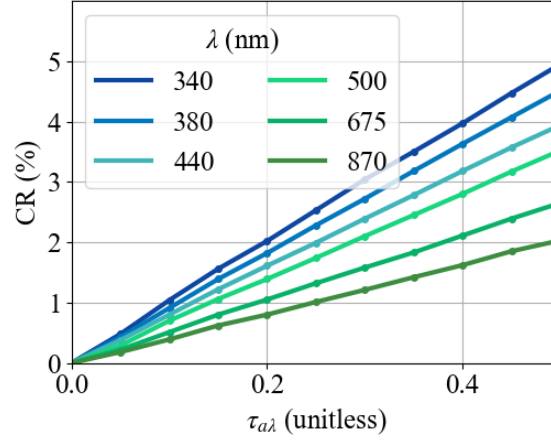


Figure 6.4: Estimated circumsolar ratio, CR (expressed as %), for an EKO MS-711 spectroradiometer, depending on the $\tau_{a\lambda}$ level, extracted from García-Cabrera et al. (2020). Figure by Paola Russo.

CIMEL sun photometers from the AERONET site at Mauna Loa Observatory or the PFR sun photometers from Global Atmospheric Watch (GAW) at the Izaña Observatory, are typically calibrated under conditions of $0.01 < \tau_{a500} < 0.02$ (Cuevas et al., 2019). In this study, the ranges of $\tau_{a\lambda}^0$ during the instants used for the calibration are shown in Table 6.3.

Table 6.3: Spectral irradiance at TOA ($G_{s,\lambda}$) used in this work. The values are obtained as the average of the Langley Plot method over short periods intervals during 2022/11/02. The number of short periods, the standard deviation, σ (expressed as percentage of $G_{s,\lambda}$) and the range of the reference $\tau_{a\lambda}^0$ (AERONET) are reported in the last three columns. * $G_{s,\lambda}$ at 340 nm was also composed with two periods from other clear days.

λ (nm)	$G_{s,\lambda}$ (W/m ² μm)	periods	σ (%)	$\tau_{a\lambda}^0$ range
340	773.4	5*	4.1	0.059-0.062
380	979.7	8	2.6	0.061-0.066
440	1605.3	8	3.1	0.054-0.059
500	1869.6	8	2.3	0.049-0.059
675	1377.3	5	2.1	0.038-0.042
870	1217.9	4	1.1	0.030-0.034

The Langley Plot method is applied to the measurements made during the clearest day selected, 2nd of November 2022, within 1-hour intervals, to obtain $G_{s,\lambda}^j$ estimates for the j^{th} interval of steady atmospheric conditions. This day is selected because it has the lowest $\tau_{a\lambda}^0$ and the highest coefficients of determination (R^2) in each period, thus the points have good alignment and small

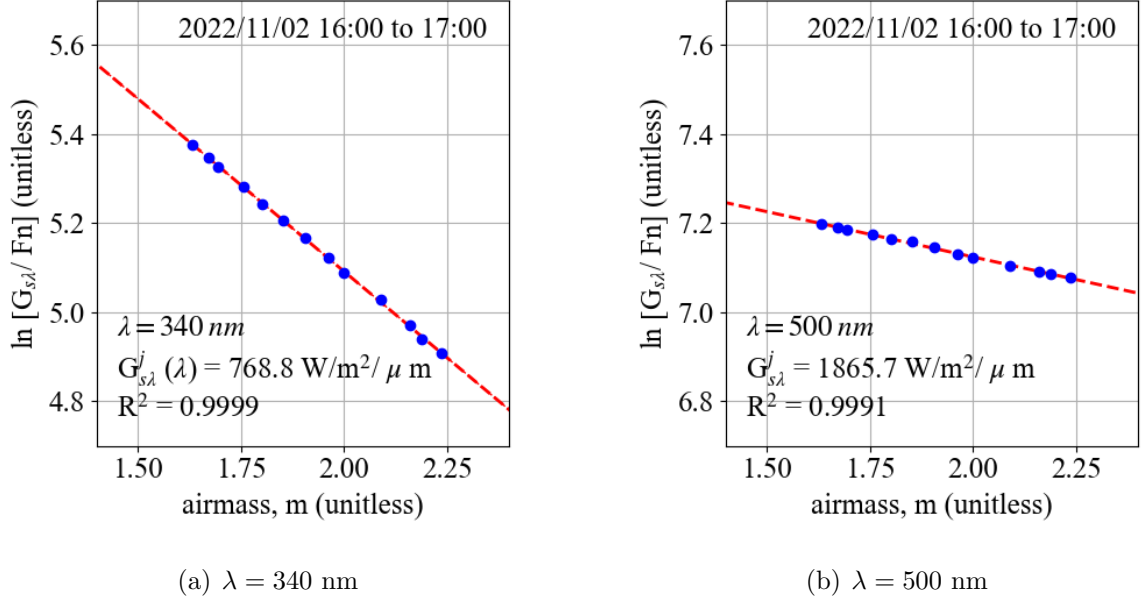


Figure 6.5: Langley plots at wavelengths = 340 and 500 nm, for one sample period. The least squares fit to the samples is shown as a red dashed line. Figure by Paola Russo.

errors in the linear regression. The Langley plots for two wavelengths in one example period, from 16:00 to 17:00 hs, are shown in Fig. 6.5. The value of $G_{s,\lambda}$ used in the inversion algorithm is the average value between the $G_{s,\lambda}^j$ obtained that had the highest coefficient of determination (R^2). The final estimates for $G_{s,\lambda}$ and their standard deviation are shown in Table 6.3.

In this chapter, the term residuals (ε), which have a value for each instant, (Eq. 6.13), will be used for referring to the difference between $\tau_{a\lambda}$ and $\tau_{a\lambda}^0$ (taking AERONET as reference):

$$\varepsilon = \tau_{a\lambda} - \tau_{a\lambda}^0. \quad (6.13)$$

For the $G_{s,\lambda}$ values to be considered acceptable, an additional criteria is used, recommended by WMO/GAW (2004), which consists of checking that the residuals comply with a U_{95} criteria (Eq. 6.14). This criteria requires that more than 95% (U_{95}) of the instants used to find $G_{s,\lambda}$, comply with the condition of their residuals being between the lower and upper limits defined in Eq. (6.14), which depend on the air mass, m_a :

$$U_{95} : |\varepsilon| < \pm(0.005 + 0.010/m_a). \quad (6.14)$$

Figure 6.6 shows the residuals obtained during the instants used for the calibration. Different colours and markers correspond to the six different wavelengths and the grey curves correspond

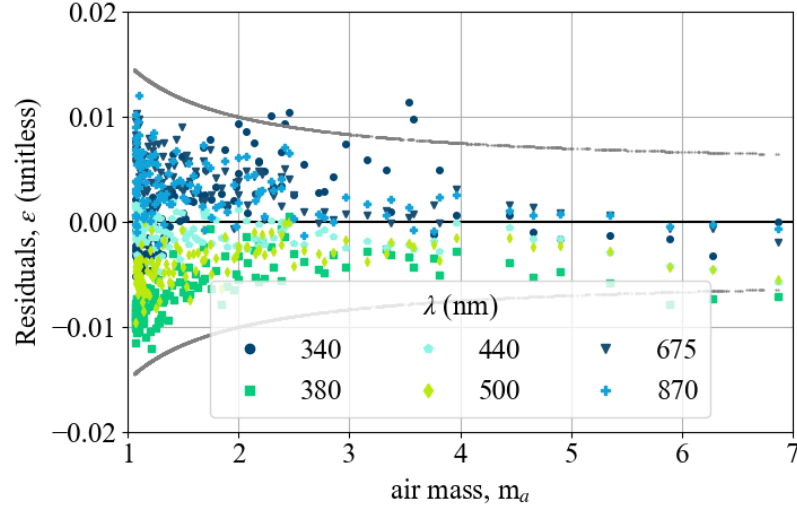


Figure 6.6: U_{95} criteria (WMO/GAW (2004), (Eq. 6.14)) applied at every wavelength, to determine if the values of $G_{s,\lambda}$ estimated return $\tau_{a\lambda}$ that fall within the U_{95} limits: $\pm(0.005 + 0.010/m_a)$, during the instants used for calibration. Figure by Paola Russo.

to the lower and upper limits of the U_{95} criteria. As a result, more than 95% of the points fall within the acceptance limits during the instants used for the calibration, denoting the good quality of the calibration instants and their suitability for calibration purposes.

The metrics used to analyse the accuracy of $\tau_{a\lambda}$ are based on the residuals Eq. (6.13). These metrics are the Mean Bias Deviation (MBD, unitless) and the Root Mean Squared Deviation (RMSD, unitless), (Eq. 2.26), described previously in Section 2.5.

The pseudo-calibration procedure makes the retrieval independent of the instrument's previous calibration.

6.2. Results

Aerosol optical depth for wavelengths 340, 380, 440, 500, 675 and 870 nm has been retrieved from 2629 spectroradiometer measurements. Performance metrics for these results are shown in Table 6.4, including in the last column the mean value from AERONET used as a reference. When the dispersion, quantified by the RMSD, is compared to other sites (as shown in Table 6.1), it is observed that its values are similar. However, some underestimation is apparent at all wavelengths.

There is a large variability in the results between different days. Therefore, Table 6.5 also shows

Table 6.4: Performance results, for the whole period (2629 instants). The last two columns show the average $\tau_{a\lambda}$ from this work and AERONET respectively.

λ (μm)	MBD (unitless)	RMSD (unitless)	$\tau_{a\lambda}$ This work	$\tau_{a\lambda}^0$ AERONET
340	-0.005	0.015	0.121	0.126
380	-0.015	0.021	0.107	0.122
440	-0.010	0.017	0.097	0.107
500	-0.013	0.019	0.082	0.095
675	-0.006	0.016	0.066	0.072
870	-0.006	0.015	0.054	0.060

the performance results for the 125 measurements of the clearest day selected (November 2nd, 2022). For this day, the dispersion is lower (RMSD below 0.007, unitless) and the bias decreases in absolute terms, but with alternating signs indicating under-estimations and over-estimations at different wavelengths, which is a good sign.

Table 6.5: Performance results for the clearest day selected: November 2nd 2022, based on 125 instants. The last two rows show the average $\tau_{a\lambda}$ from this work and AERONET respectively.

λ (μm)	MBD (unitless)	RMSD (unitless)	$\tau_{a\lambda}$ This work	$\tau_{a\lambda}^0$ AERONET
340	0.001	0.004	0.070	0.069
380	-0.006	0.007	0.066	0.072
440	-0.001	0.002	0.063	0.064
500	-0.004	0.004	0.054	0.058
675	0.004	0.005	0.050	0.046
870	0.003	0.004	0.042	0.038

Figure 6.7 shows the MBD for every wavelength with error bars of $\pm$ RMSD for the whole period (blue) and for the clearest day (green). In each case, the average MBD is indicated as a dashed horizontal line. As expected, biases for the clearest day (2022/11/02) are lower at every wavelength and their average is very close to zero. Additionally, RMSD's are also lower. Even though the low errors are partially explained because the calibration is done within that day, not every instant was taken into account to perform the calibration, and still every retrieval during that day has low dispersion. Implying stable atmospheric conditions throughout the selected day. Furthermore, the $\tau_{a\lambda}^0$ was low during that day (Table 6.5), implying an extremely clear atmosphere.

To understand why the whole period has a larger dispersion, a factor to take into account is that aerosol retrievals work with small values. Small perturbations in the systems of equations of the

algorithms can produce the effect of large errors. For this reason, when large periods of retrievals (i.e. several days) are evaluated, their dispersion tends to increase, because they incorporate the uncertainties associated to a wide variety of atmospheric conditions.

The best performance during the clearest day is found at wavelengths close to the UV (340 and 440 nm) with bias under ± 0.001 (unitless) and dispersion under 0.004 (unitless). The rest of the retrievals have acceptable performance since biases are within ± 0.006 (unitless) for all cases.

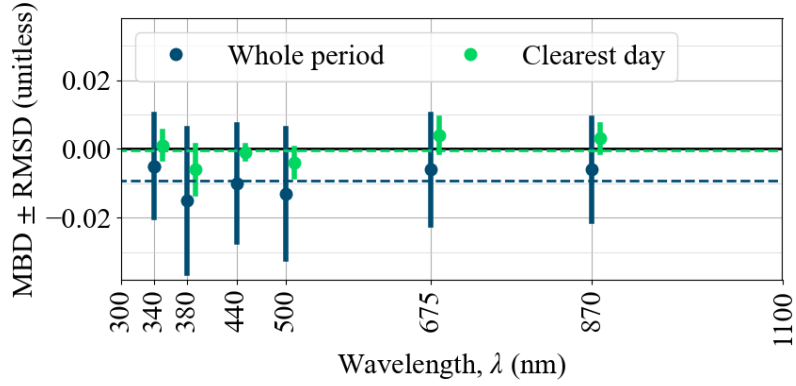


Figure 6.7: Results of MBD and RMSD for the whole period and for the clearest day. The error bars are $\pm$ RMSD (unitless). Figure by Paola Russo.

To observe the quality of the retrievals at every wavelength and during all instants, Figure 6.8 shows the scatter diagrams of $\tau_{a\lambda}$ vs. $\tau_{a\lambda}^0$. The absolute frequency is colour coded (yellow represents higher frequency) so each plot can be read as a 2D histogram. From a qualitative point of view there is a good agreement between $\tau_{a\lambda}$ retrieved and the reference $\tau_{a\lambda}^0$ from AERONET. Systematic biases are not identifiable in this case, indicating the calibration procedure and the circumsolar correction are performed correctly. There is also a soft accumulation of points around lower wavelengths since among clear-sky days it is more common to have atmospheres with low $\tau_{a\lambda}$.

Ångström Parameters

The Ångström equation (Eq. 2.23) describes approximately the dependence of $\tau_{a\lambda}$ with λ . Ångström parameters (α, β) can be estimated under stable atmospheric conditions, using $\tau_{a\lambda}$ at two or more wavelengths, because Eq. (2.23) implies a linear dependence between $\ln(\tau_{a\lambda})$ and $\ln(\lambda)$, with independent term $\ln(\beta)$ and slope $-\alpha$.

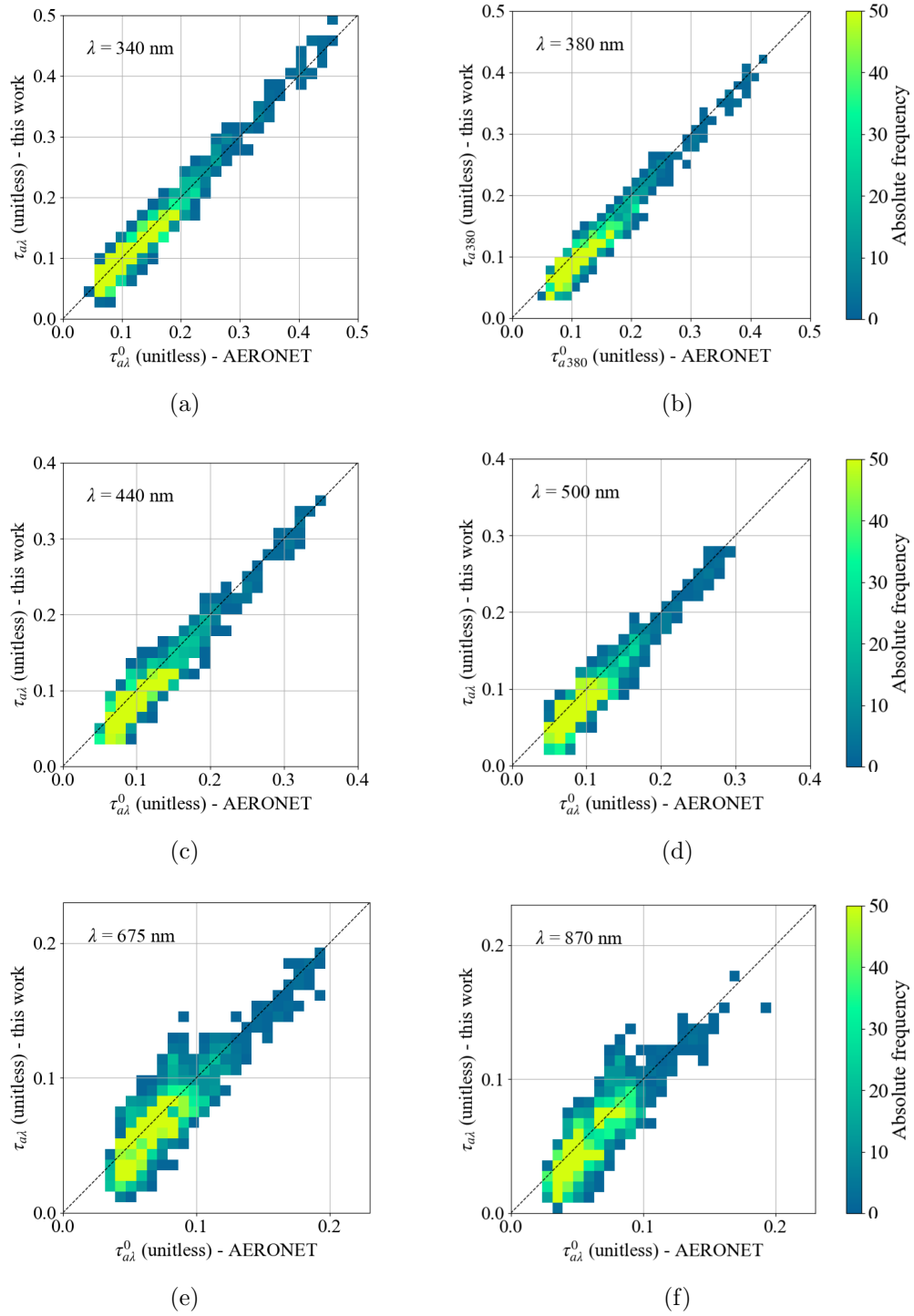


Figure 6.8: $\tau_{a\lambda}$ retrieved vs. $\tau_{a\lambda}^0$ AERONET, scatter plots with density information. Figure by Paola Russo.

The Ångström equation is first applied to the pair of aerosol optical depths: $\tau_a(\lambda = 440 \text{ nm})$ and $\tau_a(\lambda = 870 \text{ nm})$, and their corresponding wavelengths, at every instant. The slope and intercept are found by linear regression, obtaining α_i . Then α is calculated as the average for the period. This procedure is repeated for the pair of wavelengths 340-440 nm. The pairs of wavelengths chosen are intentionally coincident with the wavelengths for which AERONET reports α , to be able to compare the results taking AERONET as a reference. Additionally, the combination of wavelengths 340-440 nm and 440-870 nm is of particular interest for spectral models such as SMARTS. This wavelength range covers a wide spectral region in which typical aerosol particle sizes present in the atmosphere can be represented, helping make the aerosol model more precise. Since in this study six wavelengths are available ($\lambda = 340, 380, 440, 500, 675$ and 870 nm), the Ångström Law is also applied to all of them at once with a single linear regression.

Figure 6.9 shows the results of applying the Ångström Law in these cases. The dashed line represents the linear regression fit obtained using the estimated values of α and β . Note that when the linear regression is applied to the two points Fig. 6.9 (a and b), R^2 is obviously 1. But, when it is applied to more points Fig. 6.9 (c), obtaining an $R^2 = 0.99$, it shows how good is the agreement between the points and the estimated line. This good agreement reflects on one hand, a simple confirmation of the good quality of the samples used to perform the estimation of α and β (in this case the samples are the $\tau_{a\lambda}$ retrieved). On the other hand, having one single slope with a good agreement leads to infer that there is one main aerosol particle size and that it is in this case coarse, due to the fact that $\alpha < 1$ (Schuster et al., 2006). If there were mixed aerosol particle sizes, that is, fine mode and coarse mode coexisting, Fig. 6.9 (c) would show two well separated slopes (more as a concave curve) with a steeper slope in small wavelengths (associated to fine aerosol particles) and a flatter slope in larger wavelengths (associated with coarse aerosol particles), which is not the case.

The obtained values of α for each wavelength are compared to those reported by AERONET (Table 6.6). Column two shows α for this study and column three shows the average of the instantaneous values reported by AERONET during the same day. Note that AERONET does not report a value of α which corresponds to the regression with all wavelengths. This work presents similar values to those reported by AERONET, confirming the validity of the retrieval procedure. The estimated value for 340-440 nm is higher than the AERONET value, and for 440-870 nm it is lower, however the difference is considered to be small and related to the biases presented in $\tau_{a\lambda}$. Furthermore, it should be noted that the instantaneous values of α_i include a variability in each instant and for each wavelength, that is then transferred as uncertainty in the final averaged α .

Now that the performance of the results has been compared to the reference AERONET, values of $\tau_{a\lambda}$ and of α and β are ready to be used for practical applications. For example, they can be used to infer the type of aerosol present in the atmosphere during that period with relatively good precision and low uncertainty for this purpose. The value obtained of $\alpha = 0.535$, it is a small Ångström exponent meaning it is associated to large particles (or coarse mode aerosols),

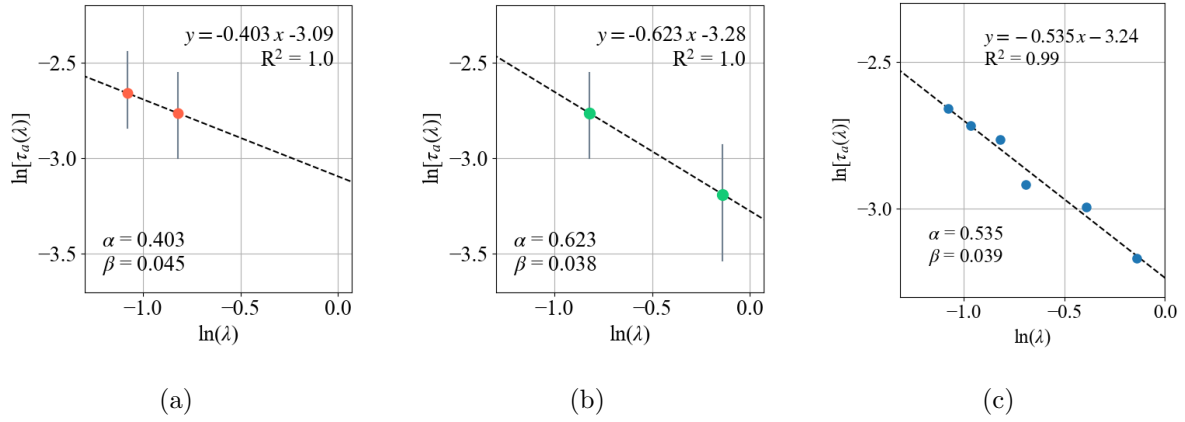


Figure 6.9: Application of the Ångström Law to find parameters α and β through linear regression, using the following wavelengths: (a) the pair $\lambda = 340\text{-}440$ nm, (b) the pair $\lambda = 440\text{-}870$ nm, (c) six wavelengths, $\lambda = 340, 380, 440, 500, 675$ and 870 nm. The dots indicate the average of $\ln[\tau_{ai}(\lambda)]$ and the vertical grey lines correspond to the minimum and maximum values of $\ln[\tau_{ai}(\lambda)]$. The day used is 2022/Nov/02, from which 125 clear sky instants have been selected. The information is related to Table 6.6. Figure by Paola Russo.

Table 6.6: Ångström exponents α from this work vs. AERONET (average for the clearest day). Note *all* corresponds to a linear regression performed with α_i from six wavelengths: 340, 440, 500, 675, 870 nm and also note that AERONET does not have a reported value of α analogous to this, as to be compared.

wavelength range (nm)	α this work	α^0 AERONET
340-440	0.403	0.319
440-870	0.623	0.762
all	0.535	—

what coincides with the site into consideration, Montevideo, which is a coastal urban site, during a period of low pollution (clear sky days), that can reasonably have aerosols of dust and sea salt (large particles) (Fig. 2.5).

6.3. Conclusions

Aerosol Optical Depth, $\tau_{a\lambda}$, at six wavelengths (340, 380, 440, 500, 675 and 870 nm) was retrieved from direct normal spectral solar irradiance measurements at a site in Uruguay over a 46-day period. Measurements were performed with an EKO MS-711 spectroradiometer, an instrument not specifically built for the retrievals purpose. The inversion algorithm was based on exponential

attenuation and applied the Langley Plot method on a selected day (2022/Nov/02) to estimate the TOA spectral irradiance. A circumsolar correction was implemented to account for the instrument's larger field of view compared to AERONET sun photometers. The retrieved $\tau_{a\lambda}$ values were compared with AERONET, showing in average, a consistent negative bias of -0.009 (MBD, unitless), and a dispersion of 0.017 (RMSD, unitless). During the calibration instants, the averaged MBD and RMSD improved to -0.001 and 0.004. These results were consistent with previous studies (Table 6.1).

It was observed that the performance of the retrieved $\tau_{a\lambda}$ is strongly influenced by the extra-terrestrial spectral irradiance estimated for the instrument, $G_{s,\lambda}$. This parameter is obtained using the Langley Plot method. Although (WMO/GAW, 2016) recommends estimating $G_{s,\lambda}$ from measurements at high-altitude sites under very stable atmospheric conditions and very low $\tau_{a\lambda}^0$, in this study the only available site for pseudo-calibration was located near sea level (56 masl). To compensate for the lack of altitude, a strict selection of calibration instants was applied, focusing on periods with low $\tau_{a\lambda}^0$ and carefully verifying clear-sky and atmospheric stability conditions. Using this approach, it was possible to estimate $G_{s,\lambda}$ at the six wavelengths and retrieve $\tau_{a\lambda}$ values that meet the U_{95} acceptability limits recommended by (Kazadzis et al., 2017; WMO/GAW, 2004). Therefore, the results are considered satisfactory for a preliminary calibration. However, it should be noted that, for full compliance with international traceability recommendations, more than 1000 measurements with τ_{a500} between 0.04 and 0.2, as well as at least five days of observations, are required.

It was noted that the performance metrics (bias and dispersion) improved significantly for a selected clear-sky day with very stable atmospheric conditions. This suggests that instants with trace cirrus clouds or variable conditions might have been selected in the broader period, and what is being observed as errors in the $\tau_{a\lambda}$ estimates, are the results of small irradiance fluctuations. Since the $\tau_{a\lambda}$ inversion algorithm is only valid for clear-sky and stable atmospheric conditions instants, it is important to precisely detect the them and discard false positives.

Regarding the circumsolar correction procedure applied, it improved $\tau_{a\lambda}$ estimates significantly, particularly in the higher $\tau_{a\lambda}$ values for each wavelength. Therefore, it is recommendable to incorporate it in retrievals based on instruments with FOV's larger than 2.5° .

The preliminary results of $\tau_{a\lambda}$ look promising. Future improvements to this methodology include correcting the negative bias, improving the clear-sky and stable atmospheric conditions selection, expanding the number of sites to other AERONET locations and comparing with other satellite data sources. In particular, the negative bias of $\tau_{a\lambda}$ estimates over all wavelengths during the period can be associated to the $G_{s,\lambda}$ estimated, which shows large uncertainties. This can be improved by using a larger set of measurements, in which more periods with clear-sky, stable atmospheric conditions and low $\tau_{a\lambda}$ become available. This problem will be addressed in future work, exploring different alternatives for the calibration methodology (Campanelli et al., 2007).

Chapter 7

Closing remarks

The overall aim of this thesis was to understand solar spectral irradiance from a physical point of view, in order to apply this knowledge in different solar resource assessment areas, such as: physical modelling of spectral and broadband irradiance under clear-sky conditions, statistical understanding of extreme events in all-sky conditions, and retrieval of atmospheric parameters from ground measurements. Different methodologies were applied and tested using ground data from two sites in Uruguay: Salto and Montevideo.

In Chapter 3, a methodology based on a threshold approach was applied to identify overirradiance events at the Salto site. Additionally, an ancillary methodology was successfully applied to detect clear-sky conditions in a broadband measured G_h time series. The analysis of overirradiance events confirmed that global solar irradiance at ground surface can temporarily exceed the theoretical clear-sky TOA irradiance of 1361 W/m^2 under specific atmospheric and cloud conditions. In that sense, during the 5 years of 1-minute samples, OI exceeded TOA irradiance in 0.2 % of the cases, reached a maximum intensity of 1601 W/m^2 in the summer of 2017, and occurred on average in 4.2 % of all samples. OIE distribution proved to be spread throughout all the seasons and during all daytimes. This finding emphasizes how important it is for solar energy applications, human health and agriculture, to account for short term variabilities. By characterizing the frequency, duration, intensity and magnitude, this work contributes to a first local understanding of extreme irradiance conditions in Uruguay that are often overlooked in conventional modelling approaches. This results not only improve the interpretation of ground based irradiance measurements but also emphasize the need to incorporate these events in models, quality control procedures and forecasting tools. Future work could link OIEs identified with this statistical method, to sky conditions classified with sky-cameras. This would improve the physical knowledge of OIEs allowing to identify what cloud configurations are most frequently associated with them.

The physical modelling of spectral and broadband irradiance under clear-sky conditions, was implemented in Chapters 4 and 5, using SMARTS and REST2 (respectively) with different sources of atmospheric information. This provided a framework on how to approach simple physical models in the region, and what performances to expect. Furthermore, an original sun and shade method was successfully used to gather both $G_{h,\lambda}$ and $G_{dh,\lambda}$ from the same global

spectroradiometer. In the case of the broadband model REST2, a rMBD as good as $\pm 1\%$ in G_h and $G_{h,PAR}$, denoted a good performance. The results were slightly worse in G_b , with a negative relative bias of -4% . The model struggled to estimate G_{dh} accurately, having a relative bias of almost 50% , what was likely explained by a bias in the atmospheric input AOD_{550} from MERRA-2. In the case of the spectral model SMARTS, its performance for G_h and G_b was also around 1% , for the best atmospheric input dataset (MODIS). SMARTS was able to estimate G_b and G_{dh} slightly better than REST2. Particularly, G_{dh} estimates from SM+MO (rMBD of 20%) outperformed those from SM+ME (rMBD of 35%) and from REST2, suggesting that G_{dh} can be improved through changes in the atmospheric inputs accuracy. Regarding spectral results, it was possible to obtain a low bias in $G_{h,\lambda}$ (around 1%) and a slightly negative bias for $G_{b,\lambda}$ (around -5%), for the best performing option (MODIS). Thus, generally speaking, the models REST2 and SMARTS proved to deliver reliable results at low computational cost, making them valuable tools for both research and operational contexts. Their relevance lies not only in the wide range of information they provide, but also in the fact that clear-sky modelling constitutes the essential foundation upon which more complex all-sky approaches are built. In parallel, the simultaneous measurement of Global, Diffuse, and Beam with a single spectroradiometer demonstrated a practical and efficient method to obtain comprehensive spectral information from a limited set of instruments. This approach is especially pertinent for monitoring stations where maximizing the utility of available equipment is critical. Together, these contributions enhance the completeness of irradiance assessments, and provide a foundation for subsequent applications, such as atmospheric components retrievals, refinement of all-sky models, and development of improved solar resource evaluation tools.

The retrieval of aerosol optical depth (AOD) from ground based beam spectral irradiance measurements was implemented in Chapter 6. It demonstrated that this parameter can be estimated with reliable accuracy, even with relative low cost instruments. In this sense, the work showed that a non dedicated instrument, such as a commercial spectroradiometer, can serve as a useful tool to monitor atmospheric AOD at several wavelengths. As results, for the six wavelengths proposed, the retrieval had an absolute MBD of -0.009 and an absolute RMSD of 0.017 in average. This results are in good general agreement with the retrievals from the reference source, AERONET. The study also addressed the challenge of operating without the possibility of calibrating the instrument at a high altitude reference station, as usually recommended in GAW protocols, and proposed an alternative to overcome this limitation, based on the use of Langley Plots. The method complied with the official U_{95} criteria for calibration of sunphotometers suggested by WMO, which validates the good quality of the samples taken and the pseudo-calibration procedure. Additionally, this work shows that accurate retrievals can be obtained for an instrument with a greater FOV than the recommended, by means of applying a circumsolar correction procedure. These results emphasize the atmospheric sensing potential of spectral irradiance measurements in regions where additional expensive equipment is not accessible and AERONET sites are sparse. Furthermore, the findings underline the capacity of spectral irradiance data to contribute simultaneously to solar resource assessment and atmospheric studies,

bridging energy oriented applications with environmental monitoring and reinforcing the versatility of physical models as essential tools to achieve this integration.

While this thesis provides insights into over-irradiance, solar irradiance physical modelling, and AOD retrievals, limitations should be acknowledged. Regarding measurement constraints, the smoothed SMARTS model was evaluated using a short data set, which allowed identification of the main performance characteristics but limits generalization. Another limitation concerns the AOD retrievals, which were relied on non dedicated instruments and alternative calibration strategies that, while effective, introduce additional uncertainties compared to standardized calibrations. Finally, long-term and seasonal variability were not comprehensively addressed, leaving scope for future work to expand both the temporal and spatial coverage. Acknowledging these limitations highlights the need for continued development and testing and justifies the methodological choices adopted in this study.

Based on the findings presented in this thesis, several directions for future research can be identified. First, expanding datasets both temporarily and geographically would provide a more comprehensive understanding of irradiance estimates. This is already being implemented for the REST2 model, in an ongoing study involving 6 stations distributed around North and South America, to be published shortly. Similarly, the SMARTS model could be applied to additional sites and longer time series. Both REST2 and SMARTS, have the potential to be used in agricultural research, as they provide detailed information on PAR irradiance, an ongoing line of work in the laboratory (DiLaccio et al., 2024). SMARTS may also contribute to current UV related research in human health (Laguarda and Abal, 2025), given its physical insight. Additionally, clear-sky physical models such as REST2 or SMARTS could be integrated into all-sky models, to represent a wider range of atmospheric conditions. This transition requires estimating the clear-sky index, a methodology previously explored for empirical models by Espino et al. (2025); Rivera-Lera et al. (2024) and potentially transferable to physical models. The study of over-irradiance events could also be enhanced through a more detailed incorporation of physical and atmospheric information; in this context, a recently acquired sky camera could be used to classify cloud cover and combine this information with statistical analyses. Atmospheric retrievals represent another emerging research direction, which could be extended to additional components such as water vapour, enabling the retrieval of multiple atmospheric products using the same instrument. Finally, the solar and atmospheric monitoring approaches described in this work could enhance the country's capabilities in modern hybrid solar–wind power plants.

In conclusion, this thesis delivers new insights and practical methodologies for the quantification of solar spectral and broadband irradiance and its interaction with the atmosphere, establishing a foundation for future regional advances in both solar energy applications and atmospheric research.

Glossary

Table 7.1: Glossary of symbols.

Symbols	Description
α (unitless)	Ångström exponent.
AOD ₅₀₀ or τ_{a500} (unitless)	Aerosol optical depth at 500 nm.
AOD ₅₅₀ or τ_{a550} (unitless)	Aerosol optical depth at 550 nm.
AOD _{λ} or $\tau_{a\lambda}$ (unitless)	Aerosol optical depth.
$A_{i\lambda}$ (unitless)	Spectral absorption coefficient of atmospheric component i .
B (unitless)	Schüepf's turbidity coefficient.
B_a (unitless)	Aerosol forward scatter factor.
β (unitless)	Ångström turbidity coefficient.
B_{Ri} (unitless)	Forward scattering fractions for Rayleigh extinction.
D (m)	Particle diameter.
Δ (min)	OIE duration.
ϵ_A (°)	EKO MS-711 collimator tube acceptance angle.
ϵ_L (°)	EKO MS-711 collimator tube limit angle.
ϵ_S (°)	EKO MS-711 collimator tube slope angle.
ϵ_{ij} (W/m ² μm)	Spectral relative residual.
ϵ_i (W/m ²) or (W/m ² μm)	Broadband or spectral residual.
F_a (unitless)	Downward scattering fraction.
F_n (unitless)	Orbital correction factor.
F_R (unitless)	SMARTS angular redistribution correction factor.
f_w (unitless)	Wavelength dependent scaling factor.
g (unitless)	Aerosol asymmetry parameter.
G_0 (W/m ²)	Solar irradiance at TOA in normal incidence.
$G_{0,\lambda}$ (W/m ² μm)	Spectral irradiance at TOA in normal incidence.
G_b (W/m ²)	Beam normal (or direct normal) irradiance.
$G_{b,\lambda}$ (W/m ² μm)	Beam normal (or direct normal) spectral irradiance.
G_{dh} (W/m ²)	Diffuse horizontal irradiance.
$G_{dh,\lambda}$ (W/m ² μm)	Diffuse horizontal spectral irradiance.

Table 7.1: Glossary of symbols.

Symbols	Description
$G_{dha,\lambda}$ (W/m ² μm)	Diffuse horiz. spectral irradiance due to aerosol scattering.
$G_{dhd,i}$ (W/m ²)	Diffuse horiz. irradiance due to back-scattering.
$G_{dh0,\lambda}$ (W/m ² μm)	Diffuse horiz. reference spectral irradiance.
$G_{dhp,i}$ (W/m ²)	Diffuse horiz. irradiance incident on a perfectly absorbing surface.
$G_{dhp,i}$ (W/m ²)	Diffuse horiz. irradiance of an ideal black surface.
$G_{dhR,\lambda}$ (W/m ² μm)	Diffuse horiz. spectral irradiance due to Rayleigh scattering.
$G_{dhs,\lambda}$ (W/m ² μm)	Diffuse horiz. spectral irradiance due to ground/background scattering.
G_h (W/m ²)	Global horizontal irradiance.
$G_{h,\lambda}$ (W/m ² μm)	Global horizontal spectral irradiance.
$G_{h,PAR}$ (W/m ²)	Global horizontal photosynthetically active radiation.
$G_{h,UV-A}$ (W/m ²)	Global horizontal UV irradiance in the range 315–400 nm.
$G_{h,UV-B}$ (W/m ²)	Global horizontal UV irradiance in the range 280–315 nm.
$G_{h,UV-C}$ (W/m ²)	Global horizontal UV irradiance in the range 110–280 nm.
$\Gamma_{o\lambda}$ (unitless)	Corrected ozone transmittance.
G_s (W/m ²)	Extraterrestrial irradiance in normal incidence at 1 A.U., or solar constant, 1361 W/m ² (Prša et al., 2016).
$G_{s,\lambda}$ (W/m ² μm)	Extraterrestrial spectral irradiance in normal incidence at 1 A.U., or reference spectrum (Wehrli, 1985).
j_λ (W m ⁻³ sr ⁻¹ μm ⁻¹)	Spectral volume coefficient.
$L_\lambda(\theta, \phi)$ (W m ⁻² sr ⁻¹ nm ⁻¹)	Spectral radiance.
$L_{a\lambda}$ (W m ⁻² sr ⁻¹ nm ⁻¹)	Spectral radiance added to the beam.
$L_{r\lambda}$ (W m ⁻² sr ⁻¹ nm ⁻¹)	Spectral radiance removed from the beam.
m (unitless)	Relative optical air mass.
M (kJ/m ²)	Over-irradiance event magnitude.
m_p (kg)	Mass of the particle.
n (m ⁻³)	Number density.
N (unitless)	Number of particles.
$n(s)$ (m ⁻³)	Number density as a function of slant path.
$n(z)$ (m ⁻³)	Number density as a function of height.
P (hPa)	Atmospheric pressure.
P_{95}	95 th percentile (Its units depend on the magnitude).
P_0 (hPa)	Standard atmospheric pressure. $P_0 = 1013.25$ hPa.
PI (W/m ²)	Over-irradiance event peak intensity.
R (m)	EKO MS-711 collimator tube field stop.
r (m)	EKO MS-711 collimator tube detector radius.
ρ (kg/m ³)	Volumetric density.

Table 7.1: Glossary of symbols.

Symbols	Description
$\rho(s)$ (kg/m ³)	Volumetric density as a function of slant path.
$\rho(z)$ (kg/m ³)	Volumetric density as a function of height.
$\rho_{b\lambda}$ (unitless)	Spectral reflectance for beam irradiance.
$\rho_{d\lambda}$ (unitless)	Spectral reflectance for diffuse irradiance.
$\rho_{s\lambda}$ (unitless)	Sky spectral reflectance.
s (m)	Slant path.
σ_{λ} (m ²)	Spectral extinction cross section.
$\sigma_{a\lambda}$ (m ²)	Spectral extinction cross section due to absorption.
$\sigma_{s\lambda}$ (m ²)	Spectral extinction cross section due to scattering.
$T_{a\lambda}$ (unitless)	Transmittance of aerosol attenuation.
$T_{aa\lambda}$ (unitless)	Transmittance of aerosol absorption.
$T_{as\lambda}$ (unitless)	Transmittance of aerosol scattering.
T_{ei} (°)	Effective temperature of atmospheric component i .
T_{ri} (°)	Reference temperature of atmospheric component i .
T_{λ} (unitless)	Transmittance.
τ_{λ} (unitless)	Total optical depth.
u_i (atm-cm)	Total path-length of atmospheric component i .
V (m ³)	Volume.
V (km)	Prevailing visibility.
VR (km)	Meteorological range.
w_0 (unitless)	Single scattering albedo of (Braslau and Dave, 1973).
w_g (unitless)	Single scattering albedo.
x (unitless)	Particle size parameter.
ξ (unitless)	Over-irradiance threshold coefficient.
z (m)	Vertical height.
θ_z (radians)	Solar zenith angle.
λ (nm)	Wavelength.
ω, Ω (steradians, st)	Solid angle.

Table 7.2: Glossary of acronyms.

Acronym	Description
TOA	Top of the atmosphere.
RTE	Radiative transfer equation.
CSR	Circumsolar radiation.
CR	Circumsolar ratio.
MBD	Mean bias deviation.
RMSD	Root mean square deviation.
OI	Over-irradiance.
OIE	Over-irradiance event.
PAR	Photosynthetically active radiation.
UV-A	Ultraviolet A.
UV-B	Ultraviolet B.
UV-C	Ultraviolet C.
FOV	Field of view.
FWHM	Full width at half maximum.
AERONET	Aerosol Robotic Network.
MODIS	Moderate Resolution Imaging Spectroradiometer.
MERRA	Modern-Era Retrospective Analysis for Research and Applications.

Units

Table 7.3: Glossary of Units

Abbreviation	Magnitude	Description
m	Longitude	meter
nm	Longitude	nanometer
μm	Longitude	micrometer
km	Longitude	kilometer
s	Time	second
msec	Time	millisecond
kg	Mass	kilogram
rad	Angle	radian
$^{\circ}$	Angle	degree
sr	Aperture	steradian (m/m)
Pa	Pressure	Pascal
$^{\circ}\text{C}$	Temperature	Celsius degrees
kg/m^2	Atmospheric columnar density	
DU	Atmospheric columnar density	Dobson Units
$\text{\AA}$	Longitude, $1 \text{ \AA} = 1 \times 10^{-10} \text{ m} = 0.1 \text{ nm}$	Ångström
A.U.	Longitude, $1 \text{ A.U.} = 149,597,870.7 \text{ km}$	Astronomical Unit

A. Appendix: Measurement instruments

A.1. EKO spectroradiometer technical description

EKO MS711 N for global horizontal spectral irradiance and EKO MS711 for direct normal spectral irradiance are grating spectroradiometers designed to measure solar spectral irradiance continuously in outdoor conditions. Its main components are described in what follows.

In the case of the instrument MS711, it has quartz window on the upper end of a collimator tube that allows it to measure specifically Direct Normal Irradiance. The collimator tube, has a slope (ϵ_S) of 1° and an aperture (ϵ_A) of 2.5° , which is half of the Field of View (FOV) of 5° . The limit angle (ϵ_L) is not specified by the manufacturer. See Figure 2.18.

The MS711-N is almost identical to the MS711-DNI, but the collimator tube is no longer there, and instead it has a hemispherical quartz dome that allows it to measure global horizontal irradiance.

Referring to the inside, a diffuser located at the bottom of the collimator tube or in the global case, in the entrance of the body, scatters the light that comes from the sun, before it enters in the slit, producing homogeneous illumination (Richter et al., 2021). In this step there is a shutter to measure the dark current.

After the light passes by the slit, it finds the Grating, designed to separate the beam of light into its component wavelengths and reflect it in the photodiode array as shown in (Fig. A.1). In the Concave Holographic Grating the light hits the curve surface in different spots with different incidence angles and in each spot it is reflected back, then it gathers at one single focal point for each wavelength and the array is then located in that focal point.

The diode array detector consists of a series of 1024 individual photodiodes and their corresponding circuits placed in a ceramic carrier, to reduce thermal effects (Agilent Technologies Inc., 2021). The diode array samples the light arriving at each photodiode, in intervals between 10 msec and 5000 msec, automatically controlled and channels the current induced by the light from each wavelength. It measures in a wavelength interval of 0.3 to 0.5 nm (to have an approximate idea, the measurements are taken in intervals of 0.43 nm near the wavelengths ranges of 300-400 nm, and intervals of 0.41 nm around the wavelength of 1100 nm).

The Point Circuit Board (PCB) receives the light and translates it into irradiance intensity. Other control devices are included in the MS711 such as a shutter to measure the dark current and a peltier to control the temperature next to the photodiode array.

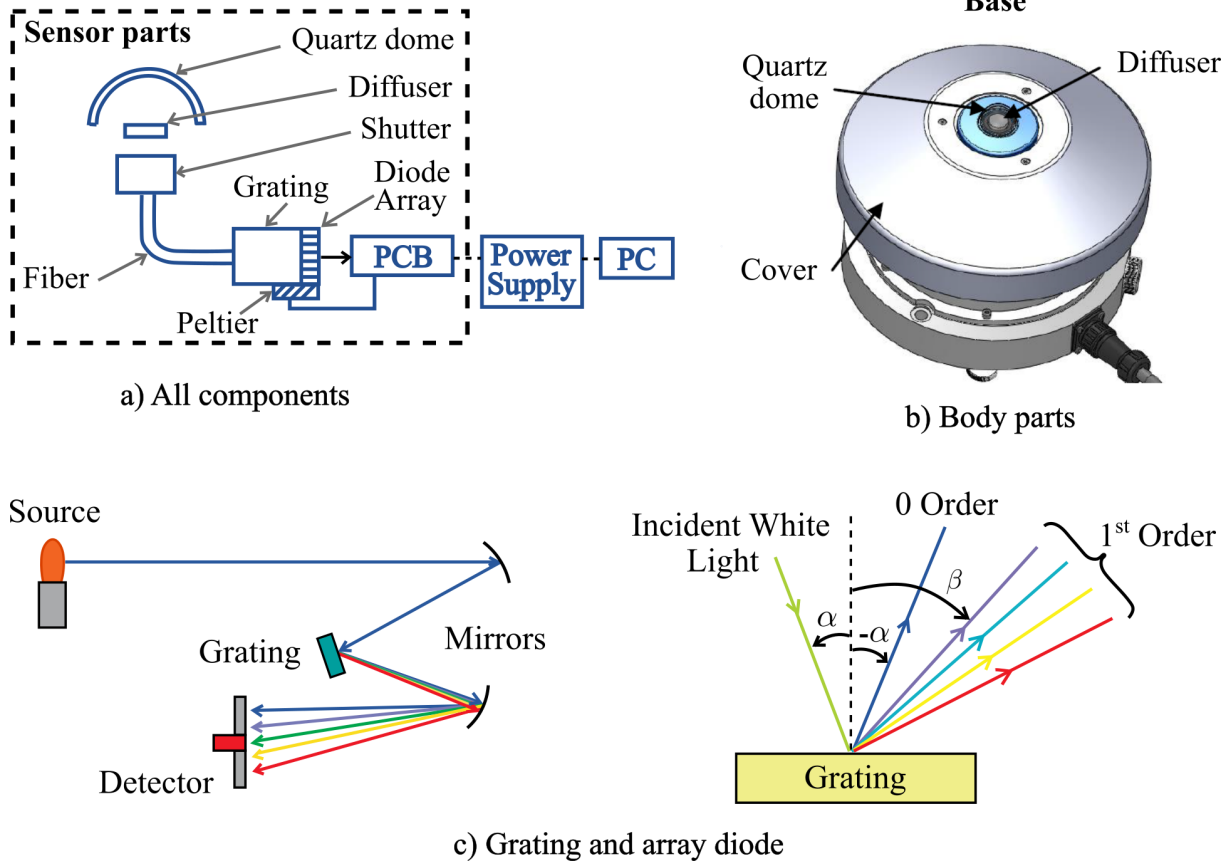


Figure A.1: Grating spectroradiometer parts and functioning principle. Adapted from Edmund Optics (2024).

A.2. Spectroradiometer traceability

Table A.1: Traceability of spectral irradiance ground measurements.

Date	Brand/Model/SN.	Description	Calibration
2020/March/23 to Present	EKO MS-711DNI sn. S19045.07	Spectroradiometer for Direct Normal Irradiance	Factory
2020/June to Present	EKO MS-711N sn. EX23062.01	Spectroradiometer for Global Horizontal Irradiance	Factory

A.3. Broadband traceability

Broadband G_h traceability

Table A.2: Traceability of ground measurements: G_h at Salto (LES) and Montevideo (AZT).

Beginning	Model/SN.	Calibration Date/Code	Cal. Factor (k) $(\frac{W}{m^2mV})$	Uncertainty (μ_k) $(\frac{W}{m^2mV})$
G_h - LES				
2016/06/19	K&Z CMP10 sn. 162966	2016/06/28 Factory	104.28	NA
2018/09/17	K&Z CMP10 sn. 140038	2018/09/17 CAL20180705	100.9	2.1
2020/10/15	K&Z CMP10 sn. 151409	2020/09/24 CAL20200924	116.1	0.9
2022/09/23- Present	K&Z CMP10 sn. 151412	2022/08/23 CAL20220805	99.3	1.2
G_h - AZT				
2015/11/24	K&Z CM11 sn. 840480	2014/12/01 NA	224.2	NA
2017/03/28	K&Z CMP11 sn. 128537	2016/06/24 CAL20160624	120.5	2.9
2018/10/31	K&Z CMP6 sn. 111916	2018/07/05 CAL20180705	101.2	2.3

Broadband G_{dh} traceability

Table A.3: Traceability of ground measurements: G_{dh} at Salto (LES).

Beginning	Model/SN.	Calibration Date/Code	Cal. Factor (k) $(\frac{W}{m^2mV})$	Uncertainty (μ_k) $(\frac{W}{m^2mV})$
G_{dh} - LES				
2016/11/19	K&Z CMP10 sn. 162967	2016/06/29 Factory	101.21	NA
2018/09/17	K&Z CMP10 sn. 162965	2018/11/27 CAL20181127	116.1	2.44
2020/10/15	K&Z CMP10 sn. 151411	2020/09/24 CAL20200924	111.4	1.1
2022/09/23- Present	K&Z CMP10 sn. 128538	2022/08/05 CAL20220805	126.2	1.4

Broadband G_b traceability

Table A.4: Traceability of ground measurements: G_b at Salto (LES).

Beginning	Model/SN.	Calibration Date/Code	Cal. Factor (k) $(\frac{W}{m^2mV})$	Uncertainty (μ_k) $(\frac{W}{m^2mV})$
G_b - LES				
2016/11/19	K&Z CHP1 sn. 120994	2012/08/30 Factory	142.27	NA
2019/05/29	K&Z CMP10 sn. 120994	2018/09/07 CAL20180907	143.47	1.1

B. Appendix: additional theoretical details

B.1. Sun-Earth distance correction factor, F_n

The Sun-Earth distance correction factor, F_n , proposed by (Spencer, 1971) is based on a Fourier parametric series, considering $\Gamma \equiv 2\pi(n-1)/365$. This expression has a maximum error of $\pm 10^{-4}$ (Iqbal, 1983).

$$F_n \approx 1.000110 + 0.034221 \cos(\Gamma) + 0.001280 \sin(\Gamma) + 0.000719 \cos(2\Gamma) + 0.000077 \sin(2\Gamma). \quad (\text{B.1})$$

B.2. Air masses related to different atmospheric processes

Air mass related to Rayleigh scattering is (Kasten and Young, 1989), with θ_z as the solar zenith angle (radians) and $\theta_{z,deg}$ as its expression in degrees,

$$m_r^{-1} = \cos \theta_z + 0.50575 \times (96.07995 - \theta_{z,deg})^{1.6364}. \quad (\text{B.2})$$

Air mass related to the NO_2 optical depth (Gueymard, 1995):

$$m_n^{-1} = \cos \theta_z + 602.30 \times \theta_{z,deg}^{0.5} (117.960 - \theta_{z,deg})^{-3.4536}. \quad (\text{B.3})$$

Air mass related to aerosols (Kasten, 1964) extinction:

$$m_a^{-1} = \cos \theta_z + 0.1500 \times (93.885 - \theta_{z,deg})^{-1.253}. \quad (\text{B.4})$$

Air mass related to Ozone (Komhyr and Grass, 1989) extinction, considering $R = 6371.229$ km is the mean radius of the Earth, $h = 22$ km is the mean height of the stratospheric ozone layer and h_s (km) is the site height above mean sea level

$$m_o = \left[1 - \left(\frac{R + h_s}{R + h} \right)^2 \sin^2 \theta_z \right]^{-1/2}. \quad (\text{B.5})$$

B.3. Air masses used specifically in REST2

Air masses specifically used in the model REST2 (Gueymard, 2008b), (Gueymard, 2003) are detailed in Eq. (B.6) and coefficients a_i are shown in Table B.1:

$$m_R^{-1} = \cos\theta_z + a_0 \theta_z^{a_1} (a_2 - \theta_z)^{a_3}. \quad (\text{B.6})$$

Table B.1: Air mass coefficients a_i used in REST2 model (Gueymard, 2008b).

	a_0	a_1	a_2	a_3
Rayleigh	4.57E-01	0.07	96.4836	-1.697
O ₃	2.68E+02	0.5	115.42	-3.2922
NO ₂	6.02E+02	0.5	117.96	-3.4536
Mix	4.57E-01	0.07	96.4836	-1.697
w	0.10648	0.11423	93.781	-1.9203
Aerosols	0.16851	0.18198	95.318	-1.9542
Kasten	0.50572	0	96.07995	-1.6364

B.4. Downward fraction of scattered radiation, F_R

The downward fraction of Rayleigh-scattered radiation, denoted as F_R (Gueymard, 1995), represents the proportion of scattered irradiance that is redirected toward the surface. It is expressed as the product of two components: $F_R = F_{R1} \times F_{R2}$. The term $F_{R1} = 0.5$ corresponds to the single-scattering approximation in a purely molecular (Rayleigh) atmosphere, assuming isotropic scattering, where half of the scattered radiation is directed downward. The factor F_{R2} introduces a correction for multiple scattering and depends on the Rayleigh optical depth, $\tau_{r\lambda}$, and the solar zenith angle, θ_z .

In Eq. (4.14), the term $F_R [1 - T_r^\lambda]$ quantifies the fraction of the horizontal extraterrestrial irradiance that, after entering the top of the atmosphere and being modulated by $\cos\theta_z$, is scattered by air molecules. Approximately half of this scattered energy (via F_{R1}) is redirected downward toward the ground, while the rest escapes to space. The F_{R2} term adjusts this fraction to account for the enhancement or reduction due to multiple scattering events.

The multiple-scattering correction factor F_{R2} is defined as:

$$F_{R2} = \begin{cases} 1 & \text{if } \tau_{r\lambda} < \tau_{rm}, \\ \exp \left\{ - \left[\left(\frac{\tau_{r\lambda} - \tau_{rm}}{\sigma_R} \right)^{0.72 + \cos\theta_z} \right] \right\} & \text{otherwise,} \end{cases} \quad (\text{B.7})$$

where the intermediate parameters are given by:

$$\sigma_R = 3.65 - 2.3 e^{-4 \cos\theta_z}, \quad \tau_{rm} = 0.17 \left[1 - e^{-8 \cos\theta_z} \right].$$

B.5. Effective ozone transmittance, $\Gamma_{0\lambda}$

The effective ozone transmittance, $\Gamma_{0\lambda}$ (Gueymard, 1995), is a parameter used to calculate diffuse radiation in SMARTS, it appears in algorithms of both, the Rayleigh component and the Aerosol scattered component. It corrects the usual ozone transmittance $T_{o\lambda}$ to take into account large errors observed in the estimation of $T_{o\lambda}$ around the UV-B region due to the supposed fact that downward diffuse irradiance depletion in that region caused by ozone does not follow the Bouguer's Law, particularly at large zenith angles.

For this reason, $\Gamma_{0\lambda}$, is calculated using an exponential decay function that changes its behaviour at $\tau_{o\lambda} = 2$:

$$\Gamma_{0\lambda} = \begin{cases} e^{-\gamma_1 \tau_{o\lambda}^{0.95} - \gamma_2 \tau_{o\lambda}} & \text{for } \tau_{o\lambda} \leq 2, \\ e^{-\gamma_3 - \gamma_4(\tau_{o\lambda} - 2)} & \text{otherwise.} \end{cases} \quad (\text{B.8})$$

Coefficients γ_1 to γ_4 are calculated as parametric expressions dependant on the relative air mass of the ozone, m_o :

$$\begin{aligned} \gamma_1 &= (-11.012 + 12.392 m_o) / (1 + 0.23644 m_o), \\ \gamma_2 &= 3.2656 \left[1 - e^{-0.46464 m_o^{1.25}} \right] - 0.965936 \gamma_1, \\ \gamma_3 &= 1.93187 \gamma_1 + 2\gamma_2, \\ \gamma_4 &= e^{0.31045 + 0.001684 m_o - 0.28549 m_o^{-4}}, \end{aligned} \quad (\text{B.9})$$

where: $\tau_{o\lambda}$ is the ozone optical depth defined in Chapter 2.

B.6. Single scattering albedo and aerosol asymmetry parameter

The single scattering albedo (ω_g , unitless, or also known as SSA), is defined as the ratio of aerosol scattering to total extinction (scattering plus absorption), as shown in (Eq. B.10). It indicates how reflective (scattering-dominant) or absorptive the aerosol particles are. SSA is a key optical property that describes the fraction of incident photons scattered by aerosols relative to the total extinction they produce. A ω_g value of 1 corresponds to a purely scattering (non-absorbing) aerosol, while lower values indicate increasing absorption. This parameter is widely used in climate modeling and radiative forcing studies, as it helps determine whether atmospheric aerosols exert a net cooling effect (by reflecting solar radiation) or a warming effect (by absorbing it). The analytic expression is given by (Gueymard, 1995):

$$\omega_g = \frac{\sigma_s}{\sigma_s + \sigma_a}, \quad (\text{B.10})$$

where σ_s (m^{-1}) is the scattering coefficient and σ_a (m^{-1}) is the absorption coefficient. These coefficients can be estimated using Mie theory (Mie, 1906) for spherical particles, or Rayleigh

scattering for very small particles, depending on their size, shape, and refractive index, as discussed in Chapter 2. Their detailed formulations are omitted, as they fall outside the scope of this work.

The aerosol asymmetry parameter, g , quantifies the mean direction of scattered light and ranges from -1 (fully backward scattering) to 1 (fully forward scattering), with values near zero indicating isotropic scattering.

B.7. Single Scattering Albedo from Braslau & Dave

One option available in SMARTS for calculating Single Scattering Albedo (w_0 , unitless) is (Braslau and Dave, 1973) parametrized formula, which depends only on the wavelength, λ :

$$w_0 = \begin{cases} 0.9941 - 0.08817 \exp(1 - 3.3815\lambda), & \text{if } \lambda < 2 \mu\text{m}, \\ 0.8569 + 0.0436\lambda, & \text{otherwise.} \end{cases} \quad (\text{B.11})$$

Table B.2: Typical Aerosol Single Scattering Albedo (ω_g) values by aerosol type, (Hess et al., 1998).

Aerosol Type	Single Scattering Albedo, ω_g
Urban / Industrial haze	0.85 – 0.92
Rural / Background	0.90 – 0.95
Maritime (sea salt)	0.98 – 1.00
Dust	0.80 – 0.90
Black carbon	0.20 – 0.40

B.8. Back scattering infinite inter reflections

Once the irradiance reaches the ground surface, if the surface is not perfectly absorbing, it will reflect a portion of the irradiance, returning it back to the atmosphere. Furthermore, scattering processes in the atmosphere can re-direct it back to the ground, and there it can be reflected again by the surface. This process can go on and on theoretically infinite times (Liou, 2002). To account for these multiple reflections, models such as SMARTS consider an infinite sum of reflection processes to obtain a final expression that will be explained below.

Consider $G_{dh0,\lambda}$ is the reference diffuse irradiance, that is the amount of diffuse solar radiation reaching the surface, assuming an ideally non-reflective surface (which means no reflection happens from the surface itself). ρ_d is the spectral reflectance of the surface for diffuse radiation and $\rho_{s\lambda}$ is the sky or atmosphere overall reflectance. Also assume an ideal situation where radiation is reflected and scattered repeatedly.

First reflection: consider the first time irradiance reaches the ground surface, the radiation that is reflected back into the atmosphere is only a portion of the initial amount. This can be expressed as:

$$\rho_{d\lambda} G_{dh0,\lambda} \quad (\text{B.12})$$

Second reflection: now this reflected irradiance is in the atmosphere, a portion of it can be scattered again by aerosols and particles present in the atmosphere, and be re directed towards the ground surface.

$$\rho_{d\lambda} \rho_{s\lambda} G_{dh0,\lambda} \quad (\text{B.13})$$

Third and n reflection: this process repeats indefinitely, and once the irradiance reaches the ground it is reflected back into the atmosphere, and so on and so forth, always returning to the ground only a scattered portion by the atmosphere.

The third time would be expressed as:

$$\rho_{d\lambda} \rho_{s\lambda}^2 G_{dh0,\lambda}. \quad (\text{B.14})$$

And the fourth as:

$$\rho_{d\lambda} \rho_{s\lambda}^3 G_{dh0,\lambda}. \quad (\text{B.15})$$

Then, the general expression that represents this process is

$$\rho_{d\lambda} \rho_{s\lambda}^{n-1} G_{dh0,\lambda}. \quad (\text{B.16})$$

Total diffuse irradiance from back-scattering: the total irradiance from all the reflections can be calculated as the sum of the infinite reflections, which mathematically, is represented by a geometric series:

$$G_{dhs,\lambda} = G_{dh0,\lambda} (\rho_{d\lambda} + \rho_{d\lambda} \rho_{s\lambda} + \rho_{d\lambda} \rho_{s\lambda}^2 + \dots + \rho_{d\lambda} \rho_{s\lambda}^{n-1}). \quad (\text{B.17})$$

Finally, knowing the result of a geometric series, the total diffuse irradiance coming from back scattering can be rewritten as:

$$G_{dhs,\lambda} = \frac{\rho_{d\lambda} G_{dh0,\lambda}}{1 - \rho_{d\lambda} \rho_{s\lambda}}. \quad (\text{B.18})$$

B.9. Parametrization coefficients for the air masses, SMARTS

Table B.3 shows the a_i coefficients used to calculate the air mass in SMARTS Gueymard (1995).

Table B.3: Coefficients a_{ix} used in the SMARTS calculation of air mass, (Eq. 4.2).

Extinction Process	a_{i1}	a_{i2}	a_{i3}	a_{i4}
Rayleigh	4.5665E-1	0.07	96.4836	-1.6970
Ozone	2.6845E+2	0.5	115.420	-3.2922
Nitrogen Dioxide	6.0230E+2	0.5	117.960	-3.4536
Mixed Gases	4.5665E-1	0.07	96.4836	-1.6970
Water Vapour	3.1141E-2	0.1	92.4710	-1.3814
Aerosols	3.1141E-2	0.1	92.4710	-1.3814

B.10. Reference atmosphere values for STS and STW in SMARTS

Table B.4 describes the values tabulated in SMARTS for the reference atmosphere profiles: Sub Tropical Summer (STS) and Sub Tropical Winter (STW). The corresponding plot is shown in Fig. 4.1.

z (km)	T (K)		P (hPa)		RH (%)	
	STS	STW	STS	STW	STS	STW
0	301.2	287.2	1013.5	1021.0	80.0	80.0
1	293.7	278.1	904.6	906.4	65.0	70.0
2	284.1	268.2	805.0	809.2	55.0	60.0
3	272.2	257.3	708.6	713.0	45.0	50.0
4	277.2	247.2	633.1	633.1	60.0	45.0
z (km)	H ₂ O (cm)		O ₃ (atm-cm)		NO ₂ (atm-cm)	
	STS	STW	STS	STW	STS	STW
0	4.219	2.101	0.300	0.250	2.00×10^{-4}	1.00×10^{-4}
1	2.593	1.206	0.292	0.336	1.88×10^{-4}	1.40×10^{-4}
2	1.506	0.744	0.365	0.364	2.17×10^{-4}	1.69×10^{-4}
3	0.884	0.439	0.359	0.380	1.72×10^{-4}	1.96×10^{-4}
4	0.604	0.269	0.320	0.369	1.95×10^{-4}	2.09×10^{-4}

Table B.4: Vertical profile of atmospheric variables and gases concentrations for STS and STW conditions. From (Gueymard, 1995).

B.11. Transmittance computation

Ozone

As an example, here it is shown how the transmittances are computed differently for each band, considering different parametrized equations. If $310 \text{ nm} < \lambda$ then:

$$\begin{aligned} c_1 &= (0.25326 - 1.7253 \lambda + 2.9285 \lambda^2)/(1 - 3.589 \lambda), \\ c_2 &= (9.6635 \times 10^{-3} - 6.3685 \times 10^{-2} \lambda + 0.10464 \lambda^2)/(1 - 3.6879 \lambda). \end{aligned} \quad (\text{B.19})$$

If $310 \leq \lambda \leq 344 \text{ nm}$:

$$\begin{aligned} c_1 &= 0.39626 - 2.3272 \lambda + 3.1476 \lambda^2, \\ c_2 &= 1.8268 \times 10^{-3} - 0.10928 \lambda + 0.16338 \lambda^2. \end{aligned} \quad (\text{B.20})$$

If $344 \leq \lambda \leq 560 \text{ nm}$:

$$A_{o\lambda}(T_{eo}) = \max \left\{ 0, A_{o\lambda}(T_{ro}) \left[1 + 0.0037083 (T_{eo} - T_{ro}) e^{28.04 (0.4474 - \lambda)} \right] \right\}. \quad (\text{B.21})$$

Nitrogen dioxide

Table B.5 shows the empirical coefficients f_i used in the computation of the Nitrogen Dioxide transmittance:

Wavelength range	f_0	f_1	f_2	f_3	f_4	f_5
$\lambda < 625 \text{ nm}$	0.69773	-8.1829	37.821	-86.136	96.615	-42.635
$\lambda \geq 625 \text{ nm}$	0.03539	-0.04985	-	-	-	-

Table B.5: Empirical coefficients f_i for different wavelength ranges, for Nitrogen Dioxide transmittance.

Water vapour

Further details on how the water vapour transmittance from Eq. (4.9) is calculated in SMARTS are presented below.

Coefficient f_w , n and c have parametric expressions that ultimately depend on the wavelength:

$$\begin{aligned} f_w &= k_w [0.394 - 0.26946\lambda + (0.46478 + 0.23757\lambda) P], \\ k_w &= \begin{cases} 1 & \text{if } \lambda \leq 0.67 \mu\text{m} \\ (0.98449 + 0.023889 \lambda) w_q & \text{otherwise,} \end{cases} \\ n &= 0.88631 + 0.025274 \lambda - 3.5949 e^{-4.5445 \lambda}, \\ c &= 0.53851 + 0.003262 \lambda + 1.5244 e^{-4.2892 \lambda}. \end{aligned} \quad (\text{B.22})$$

B_w is the band wing correction factor and its parameterized expression is:

$$B_w = h(m_w w) e^{0.1916 - 0.0785 m_w + 4.706 \times 10^{-4} m_w^2},$$

$$h(m_w w) = \begin{cases} 0.624 m_w w^{0.457} & \text{if } A_{w\lambda} < 0.01, \\ (0.525 + 0.246 m_w w)^{0.45} & \text{otherwise.} \end{cases} \quad (\text{B.23})$$

B.12. Aerosol model (Shettle & Fenn) for obtaining α_1 and α_2 depending on the relative humidity in SMARTS

To estimate α_1 and α_2 , SMARTS allows the user to choose from different pre-defined aerosol models, based on empirical coefficients published by different authors. For example, if the user chooses the aerosol model Shettle and Fenn (1979) (Table B.6) and then chooses one of its options to define the aerosol type (Rural, Urban, Maritime or Tropospheric), then depending on the relative humidity (specified as input or estimated by SMARTS), the model will estimate coefficients α_1 and α_2 as:

$$\alpha_1 = (C_1 + C_2 X_{rh}) / (1 + C_3 X_{rh}),$$

$$\alpha_2 = (D_1 + D_2 X_{rh} + D_3 X_{rh}^2) / (1 + D_4 X_{rh}). \quad (\text{B.24})$$

The parametrization that implements this is described in Eq. (B.24) and comes from a linear fit between experimental atmospheric data obtained by C. Gueymard in USA and expressions with coefficients C_i and D_i (shown in Table B.6). Consider $X_{rh} = \cos(0.9 RH)$. As an example, Fig. 4.5 shows the aerosol transmittance calculated by SMARTS for specific conditions in the 300-2300 nm wavelength range.

Table B.6: α_1 and α_2 empirical values for different relative humidities and different aerosol models.

Relative Humidity		0 %	50 %	70 %	80 %	90 %	95 %	98 %	99 %
Rural	α_1	0.933	0.932	0.928	0.902	0.844	0.804	0.721	0.659
	α_2	1.444	1.441	1.428	1.376	1.377	1.371	1.205	1.134
Urban	α_1	0.822	0.827	0.838	0.829	0.779	0.705	0.583	0.492
	α_2	1.167	1.171	1.186	1.229	1.256	1.252	1.197	1.127
Maritime	α_1	0.468	0.449	0.378	0.226	0.232	0.195	0.141	0.107
	α_2	0.626	0.598	0.508	0.286	0.246	0.175	0.098	0.053
Tropospheric	α_1	1.010	1.008	1.005	0.980	0.911	0.864	0.797	0.736
	α_2	2.389	2.379	2.357	2.262	2.130	2.058	1.962	1.881

Table B.7: Coefficients for the Shettle & Fenn aerosol model.

Coefficient	C ₁	C ₂	C ₃	D ₁	D ₂	D ₃	D ₄
Rural	0.581	16.823	17.539	0.8547	78.696	0	54.416
Urban	0.2595	33.843	39.524	1	84.254	-9.1	65.458
Maritime	0.1134	0.8941	1.0796	0.04435	1.6048	0	1.5298
Tropospheric	0.6786	13.899	13.313	1.8379	14.912	0	5.96

B.13. Full Width at Half Maximum (FWHM)

Even though analytically, spectral irradiance can be defined at a given wavelength, real spectroradiometers cannot measure the irradiance exactly at a specific wavelength, because they cannot isolate the irradiance coming from an infinitely small wavelength range that tends to zero and centers in λ . Instead, they measure in a small wavelength range (as small as possible), centered in the desired wavelength, and this continues for an array of wavelengths. The physical device that does this, for example in an EKO MS711 is a photo diode array, which captures the photons in 1024 wavelength ranges, or channels (see Appendix A.1 for more details on how the EKO MS711 works). Therefore, the actual response of the spectroradiometer, is discrete, and not continuous in λ . Every intensity recorded at each wavelength, is centered in the given wavelength, and has a band width, from which the photodiode has captured the irradiance. Additionally, the amount of channels and the band width of each channel depends on the spectroradiometer and its inner components, usually given in the equipment specifications.

To simulate the spectral response of a real spectroradiometer, SMARTS uses a Gaussian convolution method, that assumes that the instrument measures the irradiance coming from an interval of nearby wavelengths centred in λ , and then this intensity is pondered by a Gaussian function Eq. (B.25), meaning more comes from the centre and less comes from the sides, as in a Gaussian curve. Other curve options are also available in SMARTS, for instance to use a symmetrical triangular function centred in λ , but this is less common and will not be used in this work.

$$G_{b,\lambda} = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{\lambda^2}{2\sigma^2}}. \quad (\text{B.25})$$

The Full Width at Half Maximum (FWHM) defines how wide the Gaussian function mentioned is. The width of the Gaussian is controlled by the parameter σ , with the relationship:

$$FWHM = 2\sqrt{2\ln 2}\sigma. \quad (\text{B.26})$$

To summarize, SMARTS builds a Gaussian kernel with the FWHM provided by the user (in this case, it was used the value suggested by default, $FWHM = 6.5$ nm), and convolutions that kernel with the high resolution spectrum it has previously calculated (the raw output from SMARTS) to simulate what a real spectroradiometer would measure (the smoothed output from SMARTS).

B.14. PAR conversion ratio from photon flux to irradiance

A question that usually arises is why the conversion ratio (κ) from PAR photon flux ($Q_{h,PAR}$, $\mu\text{mol}/\text{m}^2 \text{ s}$) to PAR irradiance ($G_{h,PAR}$, W/m^2) is not a fixed value and rather an atmospheric conditions dependent value; and the answer is that it depends on how accurately it is modelled. Detailed information on this topic is presented in (DiLaccio et al., 2024).

The ratio between the global horizontal PAR irradiance measured at ground level, and the photon flux measured at ground level is $\kappa \left(\frac{\mu\text{mol}}{\text{J}} \right)$:

$$\kappa = \frac{Q_{h,PAR}}{G_{h,PAR}}. \quad (\text{B.27})$$

The ratio between the global horizontal PAR irradiance and the photon flux, estimated at 1 A.U., is $\kappa_0 \left(\frac{\mu\text{mol}}{\text{J}} \right)$:

$$\kappa_0 = \frac{Q_{s,PAR}}{G_{s,PAR}} = \frac{\int_{400}^{700} \frac{G_{s,\lambda}}{E_\lambda} d\lambda}{\int_{400}^{700} G_{s,\lambda} d\lambda} = \frac{\int_{400}^{700} \frac{\lambda G_{s,\lambda}}{N_A h c} d\lambda}{\int_{400}^{700} G_{s,\lambda} d\lambda}, \quad (\text{B.28})$$

where: $G_{s,PAR}$ (W/m^2) is the reference spectral irradiance at 1 A.U, $G_{s,\lambda}$ from (Wehrli, 1985), integrated in the wavelength range 400-700 nm. The wavelength dependent energy of the photons is calculated as $E_\lambda = N_A \frac{h c}{\lambda}$, $N_A = 6.022 \times 10^{23} \text{ mol}^{-1}$, where $h = 6.626 \times 10^{-34} \text{ J/s}$ is the Plank constant, $c = 3.00 \times 10^8 \text{ m/s}$ is the speed of light, and λ (m) is the wavelength. Considering this, $\kappa_0 = 4.55 \mu\text{mol}/\text{J}$, and its inverse, $\kappa_0^{-1} = 0.21964 \text{ J}/\mu\text{mol}$.

Typically, κ is approximated to the constant value of κ_0 . However, this consideration inherently assumes that the irradiance that reaches ground level is not affected by atmospheric attenuation. This conforms an acceptable simplification for applications with low precision requirements, but is not strictly true. In cases where greater precision is required, the effects of the atmosphere can be considered, and a discrimination between global horizontal, diffuse horizontal and beam normal irradiance can be applied, obtaining κ_g , κ_d and κ_b respectively. In that case, κ_g and κ_d are:

$$\kappa_g = \frac{Q_{h,PAR}}{G_{h,PAR}} = 4.57 \frac{\mu\text{mol}}{\text{J}}, \quad (\text{B.29})$$

$$\kappa_d = \frac{Q_{dh,PAR}}{G_{dh,PAR}} = 4.24 \frac{\mu\text{mol}}{\text{J}}. \quad (\text{B.30})$$

where $G_{h,PAR}$ and $G_{dh,PAR}$ calculated with the ASTM E-490¹ estimated standard spectra at ground level, for global and diffuse spectral irradiance. κ_b is estimated to have a value of $4.55 \frac{\mu\text{mol}}{\text{J}}$,

¹American Society for Testing and Materials (ASTM) E-490, <https://www.nrel.gov/grid/solar-resource/spectra-astm-e490.html>

under the hypothesis that the intensity of the beam normal spectral irradiance at ground level is approximately the same than at 1 A.U..

A more precise conversion ratio κ' that takes into account variable atmospheric conditions can be estimated, if for example, $G_{h,PAR}$ is modelled at ground level, with a spectral irradiance model such as SMARTS, and $Q_{h,PAR}$ is obtained afterwards. This allows to obtain a κ' variable with time.

C. Appendix: Additional results

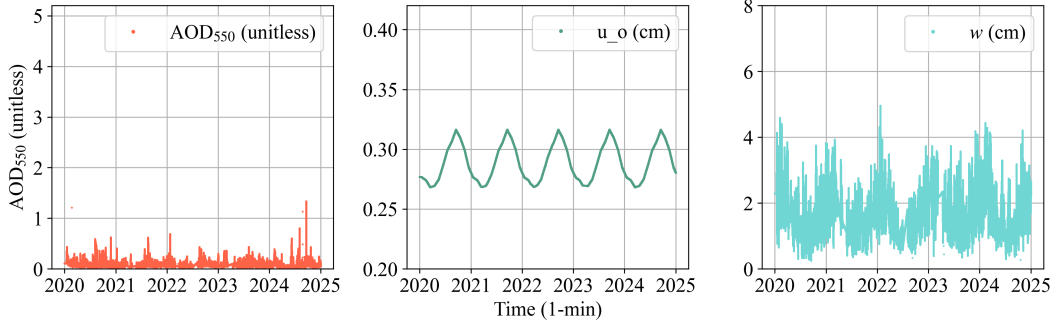
C.1. Statistics of atmospheric parameters

Table C.1 presents a brief statistical analysis of the atmospheric parameters of interest for the site Salto (DEF, MODIS/AQUA, MERRA-2) and Montevideo (AERONET) during a 5 years period (2020-01-01T00:00 to 2024-12-31T23:59) at 1 minute sampling frequency, what conforms set of 2,630,880 samples. The corresponding time series of data are shown in Table C.1. Each variable has been pre-processed by filtering extreme values that do not comply with conditions expressed in Eq. C.1 (upper and lower limits have been chosen arbitrarily considering visual inspection and physical criteria),

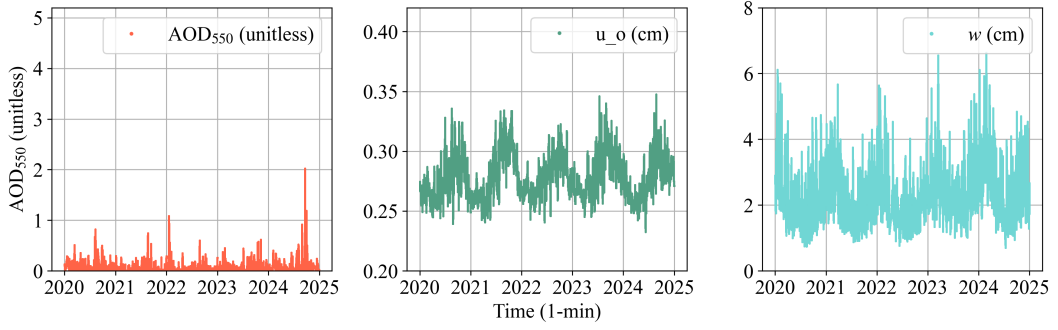
$$0 < \text{AOD}_{550} < 5, \quad 0 < w(\text{cm}) < 10, \quad 0 < u_o(\text{cm}) < 5. \quad (\text{C.1})$$

Table C.1: Minimum, average and maximum values of the atmospheric parameters for each site: Salto (Default, MODIS-AQUA and MERRA-2) and Montevideo (AERONET), during the period of 5 years, from 2020-01-01T00:00 to 2024-12-31T23:59, for 1 minute sampling frequency. The corresponding time series are shown in Fig. C.1.

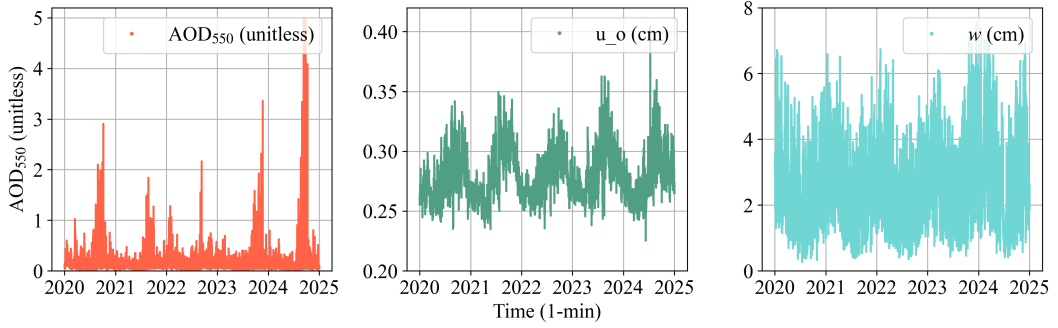
		Min	Mean	Max	std	N
DEF	AOD ₅₅₀		0.084			
	w		4.125		0	2,630,880
	u_o		0.310			
AERONET	AOD ₅₅₀	0.014	0.090	1.335	0.062	2,606,404
	w	0.248	1.713	4.967	0.726	2,622,257
	u_o	0.268	0.288	0.317	0.016	2,630,880
MODIS/AQUA	AOD ₅₅₀	0.000	0.093	2.024	0.121	2,047,299
	w	0.702	2.318	6.631	0.883	2,630,880
	u_o	0.233	0.348	2.780	0.018	2,629,620
MERRA-2	AOD ₅₅₀	0.018	0.163	4.999	0.231	2,629,697
	w	0.280	2.440	7.566	1.217	2,630,880
	u_o	0.225	0.279	0.405	0.019	2,630,880



(a) AERONET



(b) MODIS/AQUA



(c) MERRA-2

Figure C.1: Time series of atmospheric parameters from different data sources, during the period 2020-01-01 00:00 to 2024-12-31 23:59, at 1 minute frequency, for the sites Montevideo (AERONET) and Salto (MODIS/AQUA and MERRA-2). Corresponding statistics in Table C.1. Figure by Paola Russo.

C.2. Statistics of atmospheric parameters for SMARTS smoothed

For the selected samples used in the SMARTS smoothed performance study, Table C.2 shows the basic statistical measures: minimum, mean, maximum and sample standard deviation (std) of the atmospheric parameters from each data source. Table C.2 is complementary to Fig. 4.11, where time series are shown.

Table C.2: Minimum, average and maximum values of the atmospheric parameters AOD_{550} (adim), w (cm) and u_o (cm), for each data source: Default, AERONET, MODIS-AQUA and MERRA-2. Samples correspond to day 2024-06-18 from 11:15 to 13:41, which is a clear sky, stable atmospheric conditions day. The number of samples is $N = 112$. This table is corresponded with Fig. 4.11.

		Min	Mean	Max	std
DEF	AOD_{550}		0.084		
	w		4.125		0
	u_o		0.310		
AERONET	AOD_{550}	0.073	0.086	0.099	0.008
	w	2.030	2.185	2.264	0.076
	u_o	0.288	0.288	0.288	0
MODIS/AQUA	AOD_{550}	0.055	0.055	0.055	0
	w	1.653	1.691	1.726	0.022
	u_o	0.265	0.265	0.265	0
MERRA-2	AOD_{550}	0.056	0.058	0.060	0.001
	w	2.058	2.089	2.144	0.025
	u_o	0.270	0.271	0.273	0.001

C.3. Statistics of atmospheric parameters used in SMARTS raw

Table C.2 shows the minimum, average and maximum values of the atmospheric parameters for each data source: Default, AERONET, MODIS-AQUA and MERRA-2. The number of samples used for these statistics calculus is $N = 2296$ (and 2255).

Those samples are distributed in 28 days of clear sky and stable atmospheric conditions, which have been selected by rigorous visual inspection from the period 2020-01-01 to 2024-31-12. During that period, the original data set has been recorded at 1 minute frequency, containing 2,630,880 records. Once the clear sky days and periods have been selected, equally distributed into the year seasons (summer, winter, spring and autumn) and also equally distributed to represent morning, midday and afternoon, the samples go through another resampling process in order to reduce their number and make them more manageable for the purpose of modelling with SMARTS raw. To finally obtain the 2296 selected instants, a resample of 10 minutes frequency is applied (by resampling meaning picking with no aggregation included).

Table C.3: Minimum, average and maximum values of the atmospheric parameters for each data source: Default, AERONET, MODIS-AQUA and MERRA-2. The number of samples is $N = 2296$ (and 2255), equally distributed into seasons and zenith angles. They have been selected from the period 2020-01-01 to 2024-31-12, where records have originally been taken in 1 minute frequency. Fig. C.2 shows the corresponding time series.

		Min	Mean	Max	std	N
DEF	AOD ₅₅₀		0.084			
	w		4.125		0	2296
	u_o		0.310			
AERONET	AOD ₅₅₀	0.029	0.065	0.122	0.021	
	w	0.606	1.598	2.655	0.492	2255
	u_o	0.270	0.290	0.310	0.014	
MODIS/AQUA	AOD ₅₅₀	0.000	0.050	0.234	0.048	
	w	1.060	1.887	3.757	0.530	2296
	O3	0.250	0.282	0.331	0.016	
MERRA-2	AOD ₅₅₀	0.029	0.065	0.122	0.021	
	w	0.606	1.598	2.655	0.492	2296
	u_o	0.270	0.290	0.310	0.014	

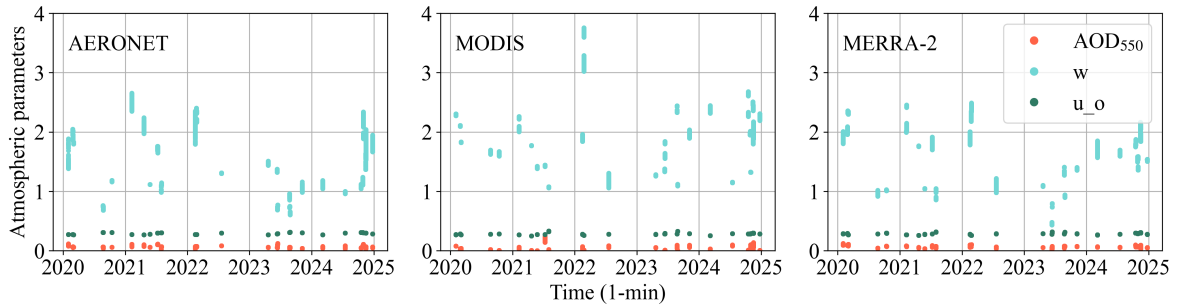


Figure C.2: Time series of the atmospheric parameters during the selected instants to analyse SMARTS broadband. Period 2020-01-01 00:00 to 2024-12-31 23:59, at 1 minute frequency, for the sites Montevideo (source: AERONET) and Salto (sources: MODIS/AQUA and MERRA-2). Corresponding statistics in Table C.3. Figure by Paola Russo.

C.4. Estimated spectroradiometer uncertainty

Having access to a quantitative value of the uncertainty of the measurement instrument allows among other things, to evaluate the performance results of the model. With this, it can be determined for example, if dispersion is close or far from the instrument's uncertainty, for a discussion on whether the performance errors are attributable to the model itself or fall within the measurements uncertainty. For this reason it is important to have an estimated value of uncertainty of the instrument. This Appendix is related to Section 4.3.2.

Uncertainty in $G_{h,\lambda}$

The uncertainty of the measurement of $G_{h,\lambda}$ is calculated here following the guides from (JCGM, 2008), identifying two uncertainties: Type A uncertainty and Type B uncertainty. Type A uncertainty corresponds to random errors introduced while measuring with the equipment, and can be estimated applying statistical analysis of a series of repeated measurements. It is, for example, signal noise. Type B uncertainty corresponds to systematic errors, it can be quantified from external sources, such as the instrument's calibration certificate. It is, for example, the calibration error, the cosine directional response and the temperature dependency. The combined uncertainty, u_c is defined as the combination of both types of uncertainties, expanded, as shown in Eq. C.2:

$$u_c(G_{h,\lambda}) = \sqrt{u_A^2 + u_B^2}. \quad (\text{C.2})$$

The typical sources of Type B uncertainty for spectroradiometers are: 1- calibration uncertainty (u_{cal}^2) 2- uncertainty due to cosine directional response (u_{dir}^2), 3- long term stability uncertainty (u_{lon}^2), 4- temperature dependence uncertainty (u_{tem}^2). It will be assumed that Type B uncertainty has a uniform statistical distribution, thus its general expression is:

$$u_B = \frac{\text{provided value}}{\sqrt{3}}. \quad (\text{C.3})$$

Uncertainty source	Reported upper limit
Calibration uncertainty	Not provided, but NIST traceable
Optical resolution (FWHM)	< 7 nm
Wavelength accuracy	± 0.2 nm
Directional response at 1000 W/m ²	< 5 %
Temperature response	< 2 % (-10°C to 50°C)

Table C.4: Manufacturer specifications for uncertainty.

Type A uncertainty is usually the repeatability uncertainty (u_{rep}^2), and can be estimated by repeating measurements under identical conditions. Assuming the conditions under which the measurements for estimating the statistical uncertainty have been done under stable atmospheric

conditions, in a very short period of time, their distribution can be assumed to be Gaussian, and then the general expression for the type A uncertainty is as Eq. C.4 shows, where s is the sample standard deviation from the n measurements,

$$u_A = \frac{s}{\sqrt{n}}. \quad (\text{C.4})$$

Combining all the sources of uncertainty mentioned (1, 2, 3, 4, 5), into Eq. C.2 leads to Eq. (C.5):

$$u_c(G_{h,\lambda}) = \sqrt{u_{rep}^2 + u_{cal}^2 + u_{dir}^2 + u_{tem}^2 + u_{lon}^2}. \quad (\text{C.5})$$

Finally, the expanded uncertainty for G_G , μ_g , is calculated as the combined uncertainty multiplied by a coverage factor, k . For a confidence value of 95 %, $k = 2$,

$$\mu_g = k \cdot u_c. \quad (\text{C.6})$$

Table C.5 shows the estimated values of uncertainty that correspond to each source. The values have been arbitrarily defined, considering a reasonable compromise between the upper limits of Table C.4 and this particular instrument conditions. u_{cal} is estimated from the National Institute of Standards and Technology (NIST, USA) reports on uncertainty (Walker et al., 1987), since the manufacturer does not provide a calibration certificate. The EKO spectroradiometers are calibrated against secondary standard spectral irradiance lamps in controlled indoor environments. These secondary standard lamps are 1000 W quartz-halogen FEL-type² lamps, traceable to primary standard lamps maintained by NIST. To ensure traceability, secondary standard lamps are calibrated in NIST laboratories following standardized procedures. During this process, they acquire transfer uncertainties ranging from 0.88 % to 2.60 %, depending on wavelength (250–2400 nm), with an average uncertainty of approximately 1 %. Consequently, spectroradiometers calibrated under these conditions are expected to inherit a measurement uncertainty of around 1 %. For u_{dir} and u_{tem} the manufacturer provides generic upper limit values published in the website³, as shown in Table C.4, in this case, they will be set to 0.5 %, a smaller value than the upper limit, because it is considered that it is more realistic. u_{lon} is set to 0.1 % since the instrument is new. u_{rep} will be estimated as 3 % uniform in the whole spectrum, since there are no measurements available taken at low frequency time intervals to calculate it (in the order of seconds). But in the future this could be improved, calculating it from real measurements, and it will probably result in a wavelength dependant value.

As an example, the calculus for a spectral irradiance of $G_{h,\lambda} = 900 \text{ W/m}^2\mu\text{m}$ is shown here.

²FEL refers to an ANSI designation, not an acronym. A FEL lamp is a quartz tungsten halogen lamp used as a reference source for calibrating photometers, colorimeters, and spectroradiometers.

³<https://eko-instruments.com/product/ms-711n-spectroradiometer/>

ID	Uncertainty source	Name	Estimated value (%)
1	Calibration	cal	1
2	Directional cosine response	dir	0.5
3	Long term stability	lon	0.1
4	Temperature dependence	tem	0.5
5	Repeatability	rep	3

Table C.5: Estimated values of uncertainty corresponding to each source.

Firstly, Type A and B uncertainties are computed, using the values estimated in Table C.5:

$$\begin{aligned}
u_{cal} &= \frac{0.01 \cdot 900}{\sqrt{3}} \approx 5.2 \text{ Wm}^{-2}/\mu\text{m}, \\
u_{dir} &= \frac{0.005 \cdot 900}{\sqrt{3}} \approx 2.6 \text{ Wm}^{-2}/\mu\text{m}, \\
u_{lon} &= \frac{0.001 \cdot 900}{\sqrt{3}} \approx 0.5 \text{ Wm}^{-2}/\mu\text{m}, \\
u_{tem} &= \frac{0.005 \cdot 900}{\sqrt{3}} \approx 5.2 \text{ Wm}^{-2}/\mu\text{m}, \\
u_{rep} &= 0.03/\sqrt{20} = 0.1 \text{ W m}^{-2}/\mu\text{m}.
\end{aligned} \tag{C.7}$$

With that, the combined uncertainty for that λ is:

$$\begin{aligned}
u_c &= \sqrt{u_{cal}^2 + u_{dir}^2 + u_{lon}^2 + u_{tem}^2 + u_{rep}^2}, \\
u_c &= \sqrt{(5.2)^2 + (2.6)^2 + (0.5)^2 + (2.6)^2 + (0.01)^2} \approx 10.9 \text{ Wm}^{-2}/\mu\text{m}.
\end{aligned}$$

And the expanded uncertainty in $G_{g,\lambda}$ is

$$\mu_g = 2 \cdot 10.9 = 21.8 \text{ Wm}^{-2}/\mu\text{m} = 2.4 \%. \tag{C.8}$$

The result of the uncertainty for an example measurement at that wavelength is reported as:

$$G_{h,\lambda} = (900 \pm 21.8) \text{ Wm}^{-2}/\mu\text{m}.$$

Uncertainty in $G_{dh,\lambda}$

Since $G_{dh,\lambda}$ is measured with the same instrument but shaded, the sources of uncertainty can be supposed the same, and from an analogous calculus, the uncertainty in $G_{dh,\lambda}$ of $900 \text{ Wm}^{-2}/\mu\text{m}$ can be estimated as:

$$\mu_d = 2 \cdot 10.9 = 21.8 \text{ Wm}^{-2}/\mu\text{m} = 2.4 \%. \tag{C.9}$$

Uncertainty in $G_{b,\lambda}$

As $G_{b,\lambda}$ is an indirect measurement, calculated from applying closure to $G_{g,\lambda}$ and $G_{dh,\lambda}$, assuming their measurements are not correlated, the uncertainty in beam (u_b) can be calculated as:

$$u_b = \sqrt{u_g^2 + u_d^2}. \quad (\text{C.10})$$

And the expanded uncertainty in beam (μ_b), using $k=2$ for a 95 % coverage factor:

$$\mu_b = 2 \cdot u_b. \quad (\text{C.11})$$

Following the previous example, it is obtained that for a $G_{b,\lambda} = 900 \text{ Wm}^{-2}/\mu\text{m}$:

$$\begin{aligned} u_b &= \sqrt{10.9^2 + 10.9^2} \approx 15.4 \text{ Wm}^{-2}/\mu\text{m}, \\ \mu_b &= 2 \cdot 15.4 = 30.9 \text{ Wm}^{-2}/\mu\text{m} = 3.4 \%. \end{aligned} \quad (\text{C.12})$$

C.5. Broadband performance of SMARTS for a single day

Table C.6: SMARTS raw spectral irradiance integrated (280-4000 nm), compared to ground measurements of G_h , G_{dh} and G_b . The table corresponds to day 2024-06-18, with 112 samples selected. The atmospheric parameters used are available in Fig. 4.11, and the corresponding plot is Fig. C.3. MBD and RMSD are shown in absolute (abs, W/m^2) and relative (rel, %) terms.

Atmos. data	Metric	G_h		G_{dh}		G_b	
		abs	rel	abs	rel	abs	rel
SMs+DE	MBD	-27.7	-5.1	27.1	41.0	-86.2	-10.2
	RMSD	27.9	5.1	27.2	41.2	86.3	10.2
SMs+AE	MBD	-6.7	-1.2	29.7	45.0	-53.3	-6.3
	RMSD	7.3	1.3	30.2	45.8	54.4	6.4
SMs+MO	MBD	6.1	1.1	16.4	24.9	-7.0	-0.8
	RMSD	6.9	1.3	16.7	25.3	7.7	0.9
SMs+ME	MBD	-0.9	-0.2	17.3	26.1	-20.9	-2.5
	RMSD	2.9	0.5	17.4	26.4	21.0	2.5
Mean Obs		547.2		66.0		846.6	

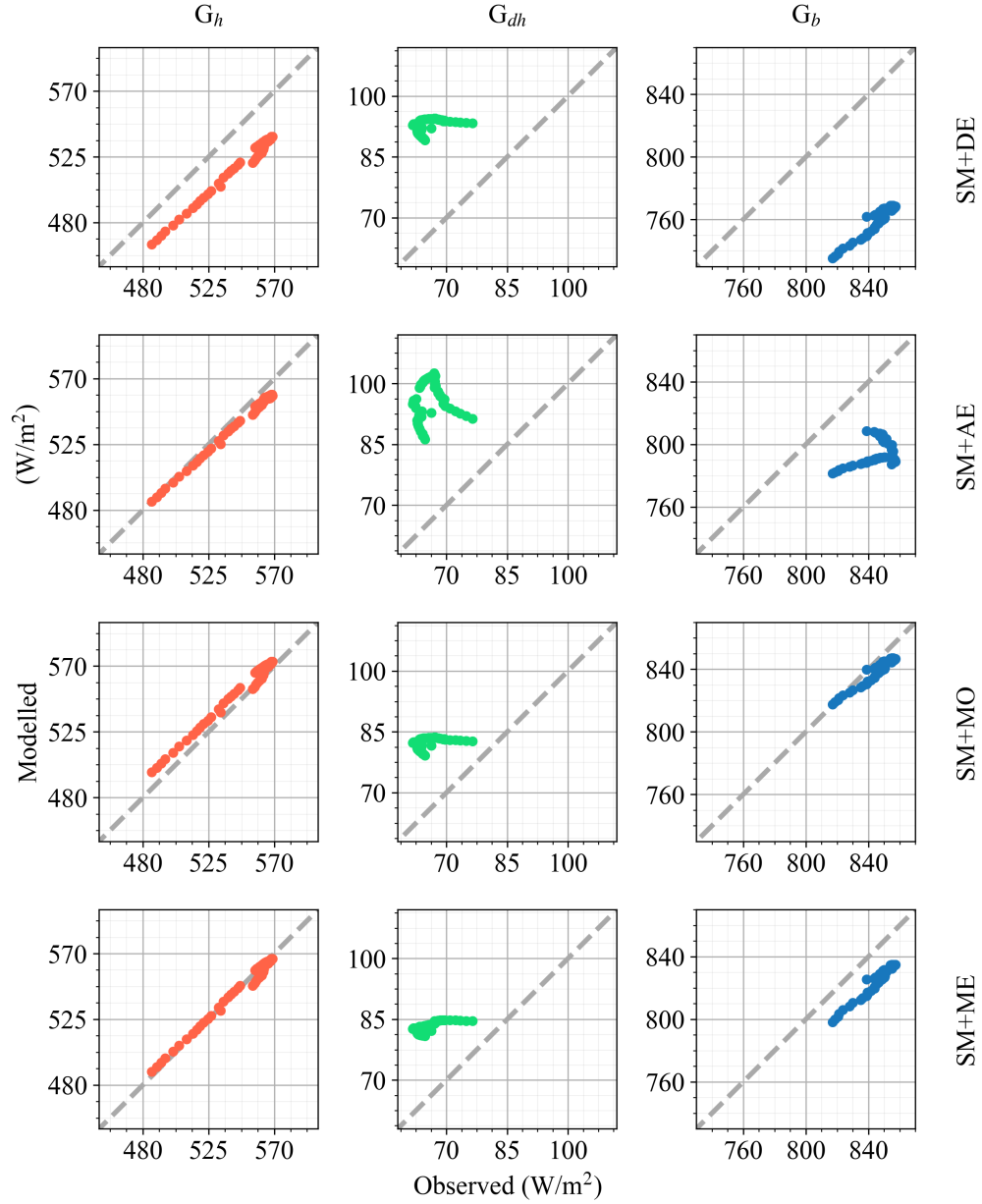


Figure C.3: Scatter plots of SMARTS raw spectral irradiance integrated (280-4000 nm), compared to ground measurements of G_h , G_{dh} and G_b . The plot corresponds to day 2024-06-18, with 112 samples selected. The atmospheric parameters used are available in Fig. 4.11 and the corresponding performance metrics are available at Table C.6. Figure by Paola Russo.

References

- Abal, G., DAngelo, M., Cataldo, J., and Gutiérrez, A. (2010). Mapa solar del Uruguay. In *Anales de la IV Conferencia Latinoamericana de Energía Solar*, Universidad Naional del Cusco, Perú. (IV ISES-CLA).
- Abreu, E. F., A., G. C., Canhoto, P., and João Costa, M. (2023). Performance assessment of clear-sky solar irradiance predictions using state-of-the-art radiation models and input atmospheric data from reanalysis or ground measurements. *Solar Energy*, 252:309–321.
- ADME (2022). Informe anual 2022. Technical report, Administracion Nacional del Mercado Electrico.
- Aggarwal, A., Kumari, R., Mehla, N., Deepali, Singh, R. P., Bhatnagar, S., Sharma, K., Sharma, K., Amit, V., and Rathi, B. (2013). Depletion of the ozone layer and its consequences: A review. *American Journal of Plant Sciences*, 4(10):1990–1997.
- Agilent Technologies Inc. (2021). Diode array detector WR and multiple wavelength detector agilent infinitylab lc series. Technical Report SD-29000218 Rev. E, Agilent InfinityLab.
- AL-agele, H., Proctor, K., Murthy, G., and Higgins, C. (2021). A case study of tomato (*solanum lycopersicon* var. legend) production and water productivity in agrivoltaic systems. *Sustainability*, 13(5).
- Alberdi, N. and Artigas, N. (2010). Viabilidad del uso de la energía solar en uruguay. Graduate thesis: Bachelor of Arts, Accountant Degree.
- Alonso-Suárez, R., Abal, G., Musé, P., and Siri, R. (2014). Satellite-derived solar irradiation map for Uruguay. In *Elsevier Energy Procedia*, volume 57, pages 1237–1246.
- Alonso-Suárez, R., Abal, G., Siri, R., and Musé, P. (2012). Brightness-dependent Tarpley model for global solar radiation estimation using GOES satellite images: application to Uruguay. *Solar Energy*, 86(11):3205–3215.

-
- Alonso-Suárez, R., D'Angelo, M., and Abal, G. (2012). Año meteorológico típico para energía solar: Región sudoeste. *Encuentro Nacional de Energías Renovables*.
- Andreas, E. (2021). The angular size of the sun. *Solar Energy*, 224:1166–1172.
- Antonanzas-Torres, F., Urraca, R., Polo, J., Perpiñán Lamigueiro, O., and Escobar, R. (2019). Clear sky solar irradiance models: A review of seventy models. *Solar Energy, Renewable and Sustainable Energy Reviews*:374–387.
- Apell, J. and McNeill, K. (2019). Updated and validated solar irradiance reference spectra for estimating environmental photodegradation rates. *Environmental Science: Processes & Impacts*, 21:427–437.
- Askar, H. and Batty, W. (2005). Assessing the performance of the “simple model of the atmospheric radiative transfer of sunshine” (smarts2) in a first tier of software using empirical weather data. *Energy*, 30(9):1577–1588.
- Atsushi, K. (2016). Importance of the green color, absorption gradient, and spectralabsorption of chloroplasts for the radiative energy balanceof leavesy. *Joournal of Solar Energy*, 9.
- Bernhard, G., Mayer, B., Seckmeyer, G., and Moise, A. (1997). Measurements of spectral solar uv irradiance in tropical-australia. *Journal of Geophysical Research: Atmospheres*, 102(D7):8719–8730.
- Bird, R. and Riordan, C. (1984). Simple solar spectral model for direct and diffuse irradiance on horizontal and tilted planes at the earth’s surface for cloudless atmospheres. Technical report, Solar Energy Research Institute (SERI), Midwest Research Institute. prepared for U.S. Department of Energy.
- Braithwaite, I., Zhang, S., Kirkbride, J., Osborn, D., and Hayes, J. (2019). Air pollution (particulate matter) exposure and associations with depression, anxiety, bipolar disorder, psychosis, and suicide risk: A systematic review and meta-analysis. *Environmental Health Perspectives*, 127(12):126002.
- Braslau, N. and Dave, J. V. (1973). Effect of aerosols on the transfer of solar energy through realistic model atmospheres. *Journal of Applied Meteorology*, 12(4):601–615.
- Bunge, C., Kruglov, R., and Poisel, H. (2006). Rayleigh and mie scattering in polymer optical fibers. *Lightwave Technology, Journal of*, 24:3137 – 3146.
- Burrows, J. P., Richter, A., Dehn, A., Deters, B., Himmelmann, S., Voigt, S., and Orphal, J. (1999). Atmospheric remote-sensing reference data from gnome-2. temperature-dependent absorption cross sections of o_3 in the 231-794nm range. *Journal of Quantitative Spectroscopy and Radiative Transfer*, 61(4):509–517.

-
- Caffaro, A. (2020). *Territorio y Energía: cambios territoriales de la Matriz Eléctrica en el Uruguay (2005 -2018)*. PhD thesis, Facultad de Ciencias Universidad de la Republica.
- Cairns, B. (1995). Diurnal variations of cloud from isccp data. *Atmospheric Research*, 37(1–3):133–146.
- Campanelli, M., Estellés, V., Tomasi, C., Nakajima, T., Malvestuto, V., and Martínez-Lozano, J. A. (2007). Application of the skyrad improved langley plot method for the in situ calibration of cimel sun-sky photometers. *Applied Optics*, 46(14):2688–2702.
- Castillejo-Cuberos, A. and Escobar, R. (2020). Detection and characterization of cloud enhancement events for solar irradiance using a model-independent, statistically-driven approach. *Solar Energy*, 209:547–567.
- Chappuis, J. (1880). Sur le spectre d’absorption de l’ozone. *Comptes Rendus de l’Académie des Sciences de Paris*, 91:985–986.
- Chen, W. T., Nenes, A., Liao, H., Adams, P., Li, J., and Seinfeld, J. (2010). Global climate response to anthropogenic aerosol indirect effects: Present day and year 2100. *Journal of Geophysical Research: Atmospheres*, 115(D12).
- Clough, S., Iacono, M., and Moncet, J. (2005). Line-by-line calculation of atmospheric fluxes and cooling rates. application to water vapor, oxygen, nitrogen, and ozone. *Journal of Geophysical Research: Atmospheres*, 110:D11104.
- Cuevas, E., Romero-Campos, P. M., Kouremeti, N., Kazadzis, S., Räisänen, P., García, R. D., Barreto, A., Guirado-Fuentes, C., Ramos, R., Toledano, C., Almansa, F., and Gröbner, J. (2019). Aerosol optical depth comparison between gaw-pfr and aeronet-cimel radiometers from long-term (2005–2015) 1 min synchronous measurements. *Atmospheric Measurement Techniques*, 12(8):4309–4337.
- Danklmayer, A. (2008). Study of tropospheric propagation effects in space-borne sar remote sensing: Latest results from terrasars-x. In *Proceedings of the ESA Workshop on Radiowave Propagation Models, Tools and Data for Space Systems*, page 4.
- de Andrade, R. and Tiba, C. (2016). Extreme global solar irradiance due to cloud enhancement in northeastern brazil. *Renewable Energy*, 86:1433–1441.
- DeBont, J., Jaganathan, S., Dahlquist, M., Persson, A., Stafoggia, M., and Ljungman, P. (2022). Ambient air pollution and cardiovascular diseases: An umbrella review of systematic reviews and meta-analyses. *Journal of Internal Medicine*, 291(6):779–800.

-
- DiLaccio, J., Russo, P., Monetta, A., Alonso-Suárez, R., and Abal, G. (2024). Atmospheric dependence of the direct, diffuse, and global clear-sky conversion ratios between solar photosynthetic active irradiance and photon flux. *Agricultural and Forest Meteorology*, 345:109832.
- Doppler, L. (2013). *Radiative transfer code development. Applications to the estimation of the radiative impact of aerosols*. PhD thesis, L’Université Pierre et Marie Curie, Berlin, Paris.
- Dubovik, O. and King, M. D. (2000). A flexible inversion algorithm for retrieval of aerosol optical properties from sun and sky radiance measurements. *Journal of Geophysical Research: Atmospheres*, 105(D16):20673–20696.
- Dubuisson, P., Dessailly, D., Vesperini, M., and Frouin, R. (2004). Water vapor retrieval over ocean using near-infrared radiometry. *Journal of Geophysical Research*, 109(D19106):1–13.
- Duffie, J. and Beckman, W. (2006). *Solar Engineering of Thermal Processes*. Wiley and Sons, Inc., Hoboken, New Jersey, third edition.
- Eck, T., Holben, B., Reid, J., Dubovik, O., Smirnov, A., O’Neill, N., Slutsker, I., and Kinne, S. (1999). Wavelength dependence of the optical depth of biomass burning, urban, and desert dust aerosols. *Journal of Geophysical Research: Atmospheres*, 104(D24):31333–31349.
- Edmund Optics (2024). Application notes, all about diffraction gratings. Electronic publication, Edmund Optics Worldwide.
- EKO, E. I. C. (2016). *Instruction Manual Grating Spectroradiometer WISER, VIS-NIR/NIR, MS-711, MS-712 MS-711*. EKO Instruments CO., Den Haag, The Netherlands.
- Emde, C., Buras-Schnell, R., Kylling, A., Mayer, B., Gasteiger, J., Hamann, U., Kylling, J., Richter, B., Pause, C., Dowling, T., and Bugliaro, L. (2016). The libradtran software package for radiative transfer calculations (version 2.0.1). *Geoscientific Model Development*, 9(5):1647–1672.
- Engerer, N. and Mills, F. (2015). Validating nine clear sky radiation models in Australia. *Solar Energy*, 120:9–24.
- Espino, B., Bove, I., and Laguarda, A. (2025). Análisis de variantes del modelo satelital semiempírico lcim para la estimación de irradiancia solar en superficie: caso de estudio en dos sitios de uruguay. *Avances en Energías Renovables y Medio Ambiente*, 28:344–355. XLVI Reunión de Trabajo de la ASADES.
- Feister, U., Cabrol, N., and Häder, D. (2015). Uv irradiance enhancements by scattering of solar radiation from clouds. *Atmosphere*, 6(8):1211–1228.

-
- Feldman, D., Collins, W., Pincus, R., Huang, X., and Chen, X. (2014). Far-infrared surface emissivity and climate. *Proceedings of the National Academy of Sciences*, 111(46).
- García-Cabrera, R. D., Cuevas-Agullo, E., Barreto, A., Cachorro, V. E., Pó, M., Ramos, R., and Hoogendijk, K. (2020). Aerosol retrievals from the eko ms-711 spectral direct irradiance measurements and corrections of the circumsolar radiation. *Atmospheric Measurement Techniques*, 13(5):2601–2621.
- Gelaro, R., McCarty, W., Suárez, M., Todling, R., Molod, A., Takacs, L., Randles, C., Darmenov, A., Bosilovich, M., Reichle, R., and Wargan, K. (2017). The modern-era retrospective analysis for research and applications, version 2 (merra-2). *Journal of Climate*, 30:5419–5454.
- Giles, D., Sinyuk, A., Sorokin, M., Schafer, J., Smirnov, A., Slutsker, I., Eck, T., Holben, B., Lewis, J., Campbell, J., Welton, E., Korkin, S., and Lyapustin, A. (2019). Advancements in the Aerosol Robotic Network (AERONET) Version 3 database – automated near-real-time quality control algorithm with improved cloud screening for sun photometer aerosol optical depth (AOD) measurements. *Atmospheric Measurement Techniques*, 12:169–209.
- Gröbner, J. and Kouremeti, N. (2019). The precision solar spectroradiometer (psr) for direct solar irradiance measurements. *Solar Energy*, 185:199–210.
- Gueymard, C. (1994). Updated transmittance functions for use in fast spectral direct beam irradiance models. In *Proceedings Solar 1994 Conference*, pages 355–360, San José, California, USA.
- Gueymard, C. (1995). SMARTS2, simple model of the atmospheric radiative transfer of sunshine: Algorithms and performance assessment. Technical Report Rep. FSEC-PF-270-95,, Florida Solar Energy Center.
- Gueymard, C. (2001). Parameterized transmittance model for direct beam and circumsolar spectral irradiance. *Solar Energy*, 71:325–346.
- Gueymard, C. (2003). Direct solar transmittance and irradiance predictions with broadband models. part I: detailed theoretical performance assessment. *Solar Energy*, 74:355–379.
- Gueymard, C. (2004). The sun’s total and spectral irradiance for solar energy applications and solar radiation models. *Solar Energy*, 76(4):423–453.
- Gueymard, C. (2005). Interdisciplinary applications of a versatile spectral solar irradiance model: A review. *Energy*, 30:1551–1576.
- Gueymard, C. (2008a). Prediction and validation of cloudless shortwave solar spectra incident on horizontal, tilted, or tracking surfaces. *Solar Energy*, 82:260–271.

-
- Gueymard, C. (2008b). REST2: High-performance solar radiation model for cloudless-sky irradiance, illuminance, and photosynthetically active radiation – validation with a benchmark dataset. *Solar Energy*, 82(3):272–285.
- Gueymard, C. (2012). Clear-sky irradiance predictions for solar resource mapping and large-scale applications: Improved validation methodology and detailed performance analysis of 18 broadband radiative models. *Solar Energy*, 86(8):2145–2169. Progress in Solar Energy 3.
- Gueymard, C. (2014). A review of validation methodologies and statistical performance indicators for modeled solar radiation data: Towards a better bankability of solar projects. *Renewable and Sustainable Energy Reviews*, 39:1024–1034.
- Gueymard, C. (2017). Cloud and albedo enhancement impacts on solar irradiance using high-frequency measurements from thermopile and photodiode radiometers. part 1: Impacts on global horizontal irradiance. *Solar Energy*, 153:755–765.
- Gueymard, C. (2018). SMARTS code, version 2.9.8 user’s manual. Technical report, Solar Consulting Services.
- Gueymard, C. (2019). The SMARTS spectral irradiance model after 25 years: New developments and validation of reference spectra. *Solar Energy*, 187:233–253.
- Gueymard, C. and Ruiz-Arias, J. (2016). Extensive worldwide validation and climate sensitivity analysis of direct irradiance predictions from 1-min global irradiance. *Solar Energy*, 128:1–30. Special issue: Progress in Solar Energy.
- Gueymard, C. and Yang, D. (2020). Worldwide validation of CAMS and MERRA-2 reanalysis aerosol optical depth products using 15 years of AERONET observations. *Atmospheric Environment*.
- Habte, A., Sengupta, M., and Lopez, A. (2017). Evaluation of the national solar radiation database (nsrdb): 1998–2015. Technical Report NREL/TP-5D00-67722, National Renewable Energy Laboratory (NREL).
- Habyarimana, E., Piccard, I., Catellani, M., De Franceschi, P., and Dall’Agata, M. (2019). Towards predictive modeling of sorghum biomass yields using fraction of absorbed photosynthetically active radiation derived from sentinel-2 satellite imagery and supervised machine learning techniques. *Agronomy*, 9:203.
- Hansen, J. E. and Travis, L. D. (1974). Light scattering in planetary atmospheres. *Space Sci. Rev.*, 16:527–610.
- Hartley, W. (1880). On the probable absorption of the solar rays by atmospheric ozone. *Chemical News*, 42:268.

-
- Hartley, W. (1889). The absorption spectrum of nitrogen dioxide. *Philosophical Transactions of the Royal Society of London*, 180:1–38.
- Hess, M., Koepke, P., and Schult, I. (1998). Optical properties of aerosols and clouds: The software package opac. *Bulletin of the American Meteorological Society*, 79(5):831–844.
- Hoff, T. and Perez, R. (2012). Modeling pv fleet output variability. *Solar Energy*, 86(8):2177–2189.
- Holben, B., Eck, T., Slutsker, I., Tanré, D., Buis, J., Setzer, A., Vermote, E., Reagan, J., Kaufman, Y., Nakajima, T., Lavenu, F., Jankowiak, I., Smirnov, A., and Gueymard, C. (1998). AERONET-A federated instrument network and data archive for aerosol characterization. *Remote Sensing of Environment*, 66:1–16.
- Holick, M. (2004). Sunlight and vitamin d for bone health and prevention of autoimmune diseases, cancers, and cardiovascular disease. *The American Journal of Clinical Nutrition*, 80(6):1678S–1688S.
- Holmgren, W., Hansen, C., and Mikofski, M. (2018). pvlib python: a python package for modeling solar energy systems. *Journal of Open Source Software*, 29:884–887.
- Huggins, W. (1890). Further observations on the ultra-violet spectra of the stars. *Proceedings of the Royal Society of London*, 48:216–220.
- Huggins, W. (1939). The absorption spectrum of nitrogen dioxide in the ultraviolet region. *Journal of the American Chemical Society*, 61:2575–2581.
- IAMAP (1986). Preliminary standard atmosphere. Technical report, International Association of Meteorology and Atmospheric Physics.
- Ichoku, C., Ichoku, C., Kaufman, Y., Remer, L., Tanré, D., and Holben, B. (2002). A spatio-temporal approach for global validation and analysis of MODIS aerosol products. *Geophysical Research Letters*, 29(12):10.1029/2001GL013205.
- Ineichen, P. and Perez, R. (2002). A new air mass independent formulation for the Linke turbidity coefficient. *Solar Energy*, 73(3):151–157.
- Inman, R., Chu, Y., and Coimbra, C. (2016). Cloud enhancement of global horizontal irradiance in california and hawaii. *Solar Energy*, 130:128–138.
- Iqbal, M. (1983). *An introduction to solar radiation*. Academic Press.
- ISO 16890-2:2022, I. S. O. (2022). Air filters for general ventilation - part 2: Measurement of fractional efficiency and air flow resistance. Electronic publication, ISO.

-
- ISO 17025:2017, I. S. O. (2017). Requisitos para la competencia de los laboratorios de ensayo y calibración. Electronic publication, UNIT-ISO/IEC.
- ISO 9060:2018(E), I. S. O. (2018). Solar energy - specification and classification of instruments for measuring hemispherical solar and direct solar radiation. Electronic publication, ISO.
- ISO 9488:2022, I. S. O. (2022). Solar energy - vocabulary. Electronic publication, ISO.
- ISO 9847:2023(E), I. S. O. (2023). Solar energy - calibration of field pyranometers by comparison to a reference pyranometer. Electronic publication, ISO.
- JCGM (2008). *Evaluation of measurement data — Guide to the expression of uncertainty in measurement*. Joint Committee for Guides in Metrology, Sèvres, France. JCGM 100:2008.
- Johannson, K. A., Balmes, J. R., and Collard, H. R. (2015). Air pollution exposure: a novel environmental risk factor for interstitial lung disease? *Chest*, 147(4):1161–1167.
- Järvelä, M., Lappalainen, K., and Valkealahti, S. (2020). Characteristics of the cloud enhancement phenomenon and pv power plants. *Solar Energy*, 196:137–145.
- Kaluba, V., Mohamad, K., and Ferrer, P. (2016). A model for hot mirror coating on solar parabolic trough receivers. *Journal of Renewable and Sustainable Energy*, 8(5):053703.
- Kaskaoutis, D. G. and Kambezidis, H. D. (2008). The role of aerosol models of the SMARTS code in predicting the spectral direct-beam irradiance in an urban area. *Renewable Energy*, 33(7):1532–1543.
- Kasten, F. (1964). Technical report 136 - a new table and approximation formula for the relative optical air mass. Physical publication, U.S. Army Material Command, Cold Regions Research and Engineering Laboratory, Hanover, New Hampshire.
- Kasten, F. (1996). The Linke Turbidity Factor based on improved values of the integral Rayleigh optical thickness. *Solar Energy*, 56(3):239–244.
- Kasten, F. and Young, A. (1989). Revised optical air mass tables and approximation formula. *Applied Optics*, 28(22):4735–4738.
- Kazadzis, S., Kouremeti, N., and Gröbner, J. (2017). Fourth wmo filter radiometer comparison (frc-iv). Technical report, Physikalisch-Meteorologisches Observatorium Davos, World Radiation Center.
- Kerker, M. (1969). *The scattering of light and other electromagnetic radiation*. Academic Press, New York, first edition.

-
- Komhyr, W. D. and Grass, R. D. (1989). Dobson spectrophotometer 83': A standard for total ozone measurements, 1962-1987. *Journal of Geophysical Research*, 94:9847–9861.
- Kopp, G. and Lean, J. (2011). A new, lower value of total solar irradiance: Evidence and climate significance. *GEOPHYSICAL RESEARCH LETTERS*, 38:L01706.
- Koschmieder, H. (1924). Theorie der horizontalen sichtweite. *Beiträge zur Physik der freien Atmosphäre*, 12:33–55.
- Krueger, O., Schenk, F., Feser, F., and Weisse, R. (2013). Inconsistencies between long-term trends in storminess derived from the 20cr reanalysis and observations. *Journal of Climate*, 26(3):868–874.
- Laguarda, A. (2021). *Modelado de la irradiancia solar sobre la superficie terrestre: Modelos físicos e híbridos utilizando información satelital sobre la Pampa Húmeda*. PhD thesis, Facultad de Ingeniería, Universidad de la República. Tesis de Doctorado en Ingeniería de la Energía.
- Laguarda, A. and Abal, G. (2017). Clear-Sky broadband irradiance: first model assessment in Uruguay. In *ISES Conference Proceedings, Solar World Congress 2017*, Solar Radiation Availability and Variability, pages 1–12.
- Laguarda, A. and Abal, G. (2019). Assessment of empirical models to estimate UV-A, UV-B and UV-E solar irradiance from ghi. *ISES Solar World Congress 2019*, 14(8).
- Laguarda, A. and Abal, G. (2020). Impacto de la incertidumbre de las variables atmosféricas de la base MERRA-2 en el modelado de la irradiancia solar en cielo despejado. *AVERMA*.
- Laguarda, A. and Abal, G. (2025). Uv index from global solar irradiance: performance according to cloudiness and air mass. *Air Quality, Atmosphere & Health*.
- Laguarda, A., Abal, G., Russo, P., and Habte, A. (2024). Estimating UV-B, uv-erithemic, and UV-A irradiances from global horizontal irradiance and MERRA-2 ozone column information. *Journal of Solar Energy Engineering*, 1(SOL-24-1042):13.
- Laguarda, A., Giacosa, G., Alonso-Suárez, R., and Abal, G. (2020). Performance of the site-adapted CAMS database and locally adjusted cloud index models for estimating global solar horizontal irradiation over the Pampa Húmeda. *Solar Energy*, 199:295–307.
- Langley, S. (1881). The invisible solar and lunar spectrum. *American Journal of Science*, 21(124):256–264.
- Lefèvre, M., Oumbe, A., Blanc, P., Espinar, B., Qu, Z., Wald, L., Homscheidt, M., and Arola, A. (2013). McClear: a new model estimating downwelling solar radiation at ground level in clear-sky conditions. *Atmospheric Measurement Techniques, European Geosciences Union*, 6:2403–2418.

-
- Levelt, P. F., van den Oord, G., Dobber, M., Malkki, A., Visser, H., de Vries, J., Stammes, P., Lundell, J., and Saari, H. (2006). The ozone monitoring instrument. *IEEE Transactions on Geoscience and Remote Sensing*, 44(5):1093–1101.
- Linke, F. (1922). Transmissions-koeffizient und trubungsfaktor. *Meteoreorological Magazine Beitrage zur Physik der Atmosphaere* Beitr, 10:91–103.
- Liou, K. (2002). *An Introduction to Atmospheric Radiation*. International geophysics series (book 84). Academic Press.
- Lorenzo, E., Moretón, R., Luque, I., Hontoria, L., and Aguilera, J. (2011). Overirradiance (cloud enhancement) events at high latitudes. *Solar Energy*, 85(3):569–577.
- Lucas, R., McMichael, A., Smith, W., and Armstrong, B. (2006). *Solar Ultraviolet Radiation: Global Burden of Disease from Solar Ultraviolet Radiation*. Number 13 in Environmental Burden of Disease Series. World Health Organization, Geneva.
- Mamajek, E., Prša, A., Torres, G., et al. (2015). Iau 2015 resolution b3 on recommended nominal conversion constants for selected solar and planetary properties. *arXiv e-prints*, arXiv:1510.07674.
- Matsumoto, K. and Yamanaka, T. (1992). The absorption spectrum of nitrogen dioxide in the 400–500 nm range. *Geophysical Research Letters*, 19:1071–1074.
- McArthur, L. (2005). Baseline surface radiation network operations manual. Technical Report WCRP-121/ WMO TD-No. 1274, World Climate Research Programme - WMO.
- McCartney, E. J. (1976). *Optics in the atmosphere*. Wiley, New York, first edition.
- Meng, Y., Tan, Y., Li, X., Cai, Y., Peng, J., and Long, Y. (2022). Building-integrated photovoltaic smart window with energy generation and conservation. *Applied Energy*, 324:119676.
- Mie, G. (1906). Beiträge zur optik trüber medien, speziell kolloidaler metallösungen. annalen der physik. *Annalen der Physik*, 3.
- Mikuška, P. (2013). Atmosférické aerosoly. Technical report, Ústav analytické chemie AV ČR, v.v.i., Brno.
- Mol, W. and Van Heerwaarden, C. (2025). Mechanisms of surface solar irradiance variability under broken clouds. *Atmospheric Chemistry and Physics*, 25:4419–4441.
- Myers, D. and Gueymard, C. (2004). Description and availability of the SMARTS spectral model for photovoltaic applications. In *Proceedings of the 49th International Symposium on Optical Science and Technology*, Denver, Colorado, USA. Society of Photo-Optical Instrumentation Engineers.

-
- Mõttus, M., Sulev, M., Frederic, B., Lopez-Lozano, R., and Noorma, A. (2011). *Photosynthetically Active Radiation: Measurement and Modeling*, pages 7970–8000. Springer.
- Nann, S. and Emery, K. (1992). Spectral effects on pv-device rating. *Solar Energy Materials and Solar Cells*, 27(3):189–216.
- Nann, S. and Riordan, C. (1991). Solar spectral irradiance under clear and cloudy skies: Measurements and a semiempirical model. *Journal of Applied Meteorology*, 30(4):447–462.
- Opáľková, M., Navrátil, M., Spunda, V., Blanc, P., and Wald, L. (2018). A database of 10 min average measurements of solar radiation and meteorological variables in ostrava, czech republic. *Earth System Science Data*, 10(2):873–846.
- Parker, W. (2016). Reanalyses and observations: What’s the difference? *Bulletin of the American Meteorological Society*, 97(9):1565–1572.
- Peixoto, J. and Oort, A. (1992). *Physics of Climate*. American Institute of Physics, New York.
- Perez, R., Ineichen, P., Moore, K., Kmiecik, M., Chain, C., George, R., F., and Vignola (2002). A new operational model for satellite-derived irradiances: description and validation. *Solar Energy*, 73:307–317.
- Perez-Astudillo, D., Bachour, D., and Martin-Pomares, L. (2018). Improved quality control protocols on solar radiation measurements. *Solar Energy*, 169:425–433.
- Piccioli, I. (2022). Modeling of Solar Irradiance on Tilted Surfaces: Impact of Direct–Diffuse Separation in Transposition Models. Master’s thesis, Universidad de la República, Facultad de Ingeniería, Montevideo, Uruguay. Magíster en Ingeniería de la Energía.
- Polo, J., Batlles, F., and Alados, I. (2012). Evaluation of enhancement events of total solar irradiance during cloudy conditions at granada, southeastern spain. *Renewable Energy*, 46:30–37.
- Polo, J., Wilbert, S., Ruiz-Arias, J., Meyer, R., Gueymard, C., Sári, M., Martín, L., Mieslinger, T., Blanc, P., Grant, I., Boland, J., Ineichen, P., Remund, J., Escobar, R., Troccoli, A., Sengupta, M., Nielsen, K., Renne, D., Geuder, N., and Cebecauer, T. (2016). Preliminary survey on site-adaptation techniques for satellite-derived and reanalysis solar radiation datasets. *Solar Energy*, 132:25–37.
- Porfirio, A. and Ceballos, J. (2013). Um método de estimativa de irradiação solar direta normal a partir de imagens de satélite geoestacionário: resultados preliminares. In *Anais XVI Simpósio Brasileiro de Sensoriamento Remoto - SBSR*, pages 6471–6479.
- PresidenciaUy (2013). Gobierno inaugurará la planta solar fotovoltaica con una inversión de 4 millones de dólares. Accessed on January 15, 2024.

-
- Prša, A., Torres, G., and Welsh, W. (2016). Nominal values for solar and planetary properties. *The Astronomical Journal*, 152(2):41.
- Pruppacher, H. and Klett, J. (1997). *Microphysics of Clouds and Precipitation*. Kluwer Academic Publishers, Dordrecht, 2 edition.
- Qiao, C., Liu, S., Huo, J., Mu, X., Wang, P., Jia, S., Fan, X., and Duan, M. (2023). Retrievals of precipitable water vapor and aerosol optical depth from direct sun measurements with eko ms711 and ms712 spectroradiometers. *Atmospheric Measurement Techniques*, 16(6):1539–1549.
- Reno, M. and Hansen, C. (2016). Identification of periods of clear sky irradiance in time series of GHI measurements. *Renewable Energy*, 90:520–531.
- Richter, F., Keim, C., Caron, J., Krauser, J., Weise, D., and Wenig, M. (2021). Prediction model for diffuser-induced spectral features in imaging spectrometers. *Atmospheric Measurement Techniques*, 14(2):1561–1571.
- Rigollier, C., Bauer, O., and Wald, L. (2000). On the clear sky model of the ESRA — European Solar Radiation Atlas — with respect to the Heliosat method. *Solar Energy*, 68(1):33–48.
- Rigollier, C., Lefevre, M., and Wald, L. (2001). Integration and exploitation of networked solar radiation databases for environment monitoring (SoDa Project). Technical report, SoDa.
- Rivera-Lera, N., Salazar, G., and Laguarda, A. (2024). Implementación del modelo lcim para la estimación de radiación solar en la superficie de salta capital y el rosario. *Avances en Energías Renovables y Medio Ambiente*, 28:332–343. XLVI Reunión de Trabajo de la ASADES.
- Rodgers, C. D. (2000). *Inverse Methods for Atmospheric Sounding: Theory and Practice*. University of Oxford, 27 Warren Street, Suite 401-402, Hackensack, USA, second edition.
- Rohde, A. (2008). Solar spectrum before and after passing through the atmosphere. Creative Commons Generic Attribution/Sharing-Equal 3.0 Licence. Accessed February, 2024.
- Rothman, L., Gamache, R., Tipping, R., Rinsland, C., Smith, M., Benner, D., Devi, V., Flaud, J., Camy-Peyret, C., Perrin, A., Goldman, A., Massie, S., Brown, L., and Toth, R. (1992). The HITRAN molecular database: Editions of 1991 and 1992. *Journal of Quantitative Spectroscopy and Radiative Transfer*, 48:469–507.
- Rothman, L., Jacquemart, D., Barbe, A., and et al. (1996). *The HITRAN 1996 molecular spectroscopic database*, volume 60. Journal of Quantitative Spectroscopy and Radiative Transfer.
- Ruiz-Arias, J. A., Gueymard, C. A., and Cebecauer, T. (2019). Direct normal irradiance modeling: Evaluating the impact on accuracy of worldwide gridded aerosol databases. *AIP Conference Proceedings*, 2126(1):190013.

-
- Russo, P., Abal, G., and Laguarda, A. (2021). Characterization of solar over-irradiance events in uruguay. In *Proceedings of the ISES Solar World Congress 2021*, <http://proceedings.ises.org/>. ISES, ISES, Germany. doi:10.18086/swc.2021.37.06.
- Russo, P., Laguarda, A., Abal, G., and Doppler, G. (2023). Aerosol optical depth from spectral direct normal irradiance measurements in montevideo, uruguay. *The International Archives of the Photogrammetry Remote Sensing and Spatial Information Sciences*, XLVIII-M-1:565–572.
- Russo, P., Laguarda, A., Abal, G., and Piccioli, I. (2022). Performance of the REST2 model for 1-minute clear-sky solar irradiance with merra-2 atmospheric inputs. In *Proceedings of the CBENS Congresso Brasileiro de Energia Solar 2022, Florianopolis, Brazil*, Solar Resource Assessment.
- Salmon, A., Quiñones, G., Soto, G., Polo, J., Gueymard, C., Ibarra, M., Cardemil, J., Escobar, R., and Marzo, A. (2021). Advances in aerosol optical depth evaluation from broadband direct normal irradiance measurements. *Solar Energy*, 221:206–217.
- Salomonson, V., Barnes, W., Maymon, P., Montgomery, H., and Ostrow, H. (1989). MODIS: Advanced facility instrument for studies of the Earth as a system. *IEEE Transactions on Geoscience and Remote Sensing*, 27(2):145–153.
- Salto Grande (1997). Salto grande: un símbolo de unión entre dos países. Accessed on January 15, 2024.
- Sani, M., Salihu, R., Bello, T., and Yerima, S. (2024). Validation of Multiple Satellite Aerosol Optical Depth Retrievals Using Ground-Based AERONET AOD Data over West Africa. *EGU General Assembly 2024*.
- Schuster, G., Dubovik, O., and Holben, B. (2006). Angstrom exponent and bimodal aerosol size distributions. *Journal of Geophysical Research*, 111:D07207.
- Seinfeld, J. H., Bretherton, C., Carslaw, K. S., Coe, H., DeMott, P. J., Dunlea, E. J., Feingold, G., Ghan, S., Guenther, A. B., Kahn, R., Kraucunas, I., Kreidenweis, S. M., Molina, M. J., Nenes, A., Penner, J. E., Prather, K. A., Ramanathan, V., Ramaswamy, V., Rasch, P. J., Ravishankara, A. R., Rosenfeld, D., Stephens, G., and Wood, R. (2016). Improving our fundamental understanding of the role of aerosol-cloud interactions in the climate system. *Proceedings of the National Academy of Sciences*, 113(21):5781–5790.
- Shamachurn, H. and Betts, T. (2016). Experimental study of the degradation of silicon photovoltaic devices under ultraviolet radiation exposure. *Journal of Solar Energy*, 9.
- Shaw, G. E. (1983). Sun photometry. *Bulletin of the American Meteorological Society*, 64(1):4 – 10.

-
- Shettle, E. P. and Fenn, R. W. (1979). Models for the aerosols of the lower atmosphere and the effects of humidity variations on their optical properties. Technical report, Air Force Geophysics Laboratory, USAF.
- Skartveit, A. and Olseth, J. (1988). Some simple formulas for multiple rayleigh scattered irradiance. *Solar Energy*, 41(1).
- Spencer, J. W. (1971). Fourier series representation of the position of the sun. *Search*, 2(5):172.
- Strutt, W. (1871). On the light from the sky, its polarization and colour. *Philosophical Magazine*, 41:107–120.
- Stull, R. (1988). *An Introduction to Boundary Layer Meteorology*, volume 13 of *Atmospheric Sciences Library*. Springer, Dordrecht, Netherlands.
- Thorne, P., Allan, R., Ashcroft, L., Brohan, P., Dunn, R., Menne, M., Pearce, P., Pfenninger, S., Willett, K., and Brönnimann, S. (2017). Toward a formal framework for evaluating observational uncertainty: Progress, challenges, and opportunities. *Wiley Interdisciplinary Reviews: Climate Change*, 8(1):e654.
- Toreti, L., Arns, G., and Rambo, C. (2021). Overirradiance effect on the electrical performance of photovoltaic systems of different inverter sizing factors. *Solar Energy*, 225:561–568.
- United Nations (2015). The paris agreement. Technical report, United Nations Framework Convention on Climate Change (UNFCCC).
- UruguayXXI (2022). Uruguay is at the forefront in the use of renewable energy sources. Accessed on January 15, 2024.
- UruguayXXI (2023). Compañía chilena concretará millonaria inversión en uruguay para producir ecombustibles a partir de hidrógeno verde. Accessed on January 15, 2024.
- Utrillas, M., Bosca, J., Martínez-Lozano, J., Cañada, J., Tena, F., and Pinazo, J. (1998). A comparative study of SPCTRAL2 and SMARTS2 parameterised models based on spectral irradiance measurements at valencia, spain. *Solar Energy*, 63(3):161–171.
- Utrillas, M., Martínez-Lozano, J., Cachorro, V., Tena, F., and Hernandez, S. (2000). Comparison of aerosol optical thickness retrieval from spectroradiometer measurements and from two radiative transfer models. *Solar Energy*, 68(2):197–205.
- van de Hulst, H. (1957). *Light Scattering by Small Particles*. John Wiley & Sons, New York. Reprinted by Dover Publications, New York, 1981.

-
- Vasilkov, A. P., Joiner, J., Oreopoulos, L., Gleason, J. F., Veefkind, P., Bucsela, E., Celarier, E. A., Spurr, R. J. D., and Platnick, S. (2009). Impact of tropospheric nitrogen dioxide on the regional radiation budget. *Atmospheric Chemistry and Physics*, 9(17):6389–6400.
- Waiter, A. (2019). *Trayectoria tecnológica, capacidades nacionales y aspectos institucionales: la construcción de la represa hidroeléctrica en Rincón del Bonete, Uruguay 1904-1945*. PhD thesis, Facultad de Ciencias Sociales Universidad de la República.
- Wald, L. (2020). *Fundamentals of Solar Radiation*. Taylor and Francis, Schipholweg 107C, 2316 XC Leiden, The Netherlands, first edition.
- Walker, J. H., Saunders, R. D., Jackson, J. K., and McSparron, D. A. (1987). NBS measurement services: Spectral Irradiance Calibrations. National Bureau of Standards, USA.
- Webb, A., Kline, L., and Holick, M. (1988). Influence of season and latitude on the cutaneous synthesis of vitamin d3: exposure to winter sunlight in boston and edmonton will not promote vitamin d3 synthesis in human skin. *Science*, 240(4858):1314–1316.
- Wehrli, C. (1985). Extraterrestrial solar spectrum. Technical Report no. 615, Physikalisches-Meteorologisches Observatorium and World Radiation Center.
- WMO/GAW, W. M. O. (2004). WMO/GAW experts workshop on a global surface-based network for long term observations of column aerosol optical properties. Technical Report 162, WMO/GAW.
- WMO/GAW, W. M. O. (2016). Aerosol measurement procedures, guidelines and recommendations. Technical report, World Meteorological Organization and Global Atmospheric Watch.
- World Meteorological Organization, editor (2018). *Guide to Meteorological Instruments and Methods of Observation*. Number WMO-No. 8 in WMO Technical Regulations. World Meteorological Organization, 2018 edition.
- World Meteorological Organization (WMO) (2023). *Guide to Instruments and Methods of Observation*. WMO-No. 8. WMO, Geneva.
- Young, A. (1994). Air mass and refraction. *Applied Optics*, 33(6):1108–1110.
- Zhang, X., Yin, Z., Xiang, S., Yan, H., and Tian, H. (2024). Degradation of polymer materials in the environment and its impact on the health of experimental animals: A review. *Polymers*, 16(19).
- Zhao, N. et al. (2014). Over-irradiance events and their impact on pv systems at high latitudes. In *Energy Procedia*, volume 57, pages 1232–1241.

List of Tables

2.1.	Wavelength bands as adopted in this work. The last column f_b , shows each band's fraction of total solar irradiance, according to Wehrli (1985).	10
2.2.	Coordinates and altitude of the sites for ground measurements. Note $G_{h,\lambda}$ and $G_{dh,\lambda}$ are measured with the same instrument with a methodology described in Sec. 4.2.1.	23
2.3.	Validation of MERRA-2 atmospheric variables for the Pampa Húmeda region against three AERONET sites, hourly. See (Laguarda and Abal, 2020) for the details.	29
3.1.	Filtered samples by quality control procedure (QC) and solar altitude. The percentages relative to the diurnal samples are shown in the last column.	36
3.2.	Performance of original and site adapted G_h estimates of ESRA clear sky model implemented for the work. % relative to the average of 397,622 clear-sky measurements = 624.6 W/m^2	37
3.3.	Seasonal characteristics of OI events.	40
3.4.	Number of OIE and its P_{95} duration by season and year. The year in which each variable records a maximum is highlighted in gray.	42
4.1.	Atmospheric processes that cause attenuation considered by SMARTS.	49
4.2.	Broadband performance of SMARTS G_h , G_{dh} and G_b estimates expressed as a % of the average measured G_h . The metrics are defined in Eq. (2.26). The data sources are abbreviated as: Sa21: Salmon et al. (2021), RA19: Ruiz-Arias et al. (2019), Ab23: Abreu et al. (2023), As5: Askar and Batty (2005). Atmospheric data sources are abbreviated as: AERONET (AERO), MERRA-2 (ME-2), Copernicus Atmospheric Service (CAMS). Climatic classifications according to Köpen Geiger (Prša et al., 2016).	63
4.3.	Summary of SMARTS spectral comparisons from Apell and McNeill (2019). . . .	64
4.4.	Performance metrics of SMARTS estimates in Valencia, Spain (Utrillas et al., 1998). .	64

4.5.	Performance of G_b from SMARTS v2.9.2 discriminated by spectral bands, when using different aerosol models in Athens, Greece (Kaskaoutis and Kambezidis, 2008). Spectral performance indicators are based on the relative residuals, as defined in Eq. (2.31). rMBD and rRMSD are expressed in percentage (%) relative to the mean observed values.	65
4.6.	Composite models abbreviations.	70
4.7.	Summary of the data sources available for atmospheric parameters.	71
4.8.	Summary of the variable names of each data source. The url's of access are: https://aeronet.gsfc.nasa.gov/new_web/units.html , https://giovanni.gsfc.nasa.gov	71
4.9.	Sensitivity of SMARTS to changes in input variables, for instant 2022/01/11 at 12:00 (UTC-3), Salto. $G_{b,\lambda}^+$ corresponds to a decrease in x_0 , and $G_{b,\lambda}^-$ corresponds to an increase in x_0 . The spectral variation δG_b is calculated with Eq. (4.21). . .	75
4.10.	Performance metrics (Eq. 2.28) for SMs+DE, SMs+AE, SMs+MO, SMs+ME, per wavelength range. The MBD and RMSD are expressed in relative terms (rel, %) and absolute terms (abs, $\text{W/m}^2/\mu\text{m}$) and the observed mean in ($\text{W/m}^2/\mu\text{m}$). . .	83
4.11.	Expanded uncertainty, μ	85
4.12.	Performance metrics of the SMARTS composite models (integrated over 280-4000 nm). MBD and RMSD are presented in absolute terms (abs, W/m^2) and relative terms (rel, %) as percentage of the observed mean (last row, in W/m^2). Fig. 4.19 represents these results. Based on 2249 samples.	87
5.1.	Performance metrics for REST2 estimates at 1-minute level on previous validations worldwide. rMBD and rRMSD are expressed as % of the average of the measurements. To convert into absolute values, only (Gueymard, 2012) provides the mean observed values, which are in average: $G_h = 675.6 \text{ W/m}^2$, $G_{dh} = 97.3 \text{ W/m}^2$ and $G_b = 856.8 \text{ W/m}^2$	94
5.2.	Performance metrics for REST2 estimates on previous regional validations. rMBD and rRMSD are expressed as % of the average of the measurements.	95
5.3.	Quality control and clear-sky detection results for each variable. The first row shows the number of valid data points. The second row indicates the number of data flagged by quality control (QC), also expressed as a percentage of the valid data. The third row presents the number of clear-sky samples selected, with percentages also relative to the valid data (first row).	97
5.4.	Performance metrics for REST2 estimates.	99
6.1.	Comparison of retrieved $\tau_{a\lambda}$ from EKO MS-711 measurements against AERONET estimates: García-Cabrera et al. (2020) - GC, Qiao et al. (2023) - Q. Performance is evaluated with the mean bias deviation (MBD, unitless) and the root mean squared deviation (RMSD, unitless), relative to the reference mean values. . . .	103
6.2.	Relevant optical depths considered in Eq. (6.1), for each wavelength of study. . .	106

6.3.	Spectral irradiance at TOA ($G_{s,\lambda}$) used in this work. The values are obtained as the average of the Langley Plot method over short periods intervals during 2022/11/02. The number of short periods, the standard deviation, σ (expressed as percentage of $G_{s,\lambda}$) and the range of the reference $\tau_{a\lambda}^0$ (AERONET) are reported in the last three columns. $*G_{s,\lambda}$ at 340 nm was also composed with two periods from other clear days.	109
6.4.	Performance results, for the whole period (2629 instants). The last two columns show the average $\tau_{a\lambda}$ from this work and AERONET respectively.	112
6.5.	Performance results for the clearest day selected: November 2 nd 2022, based on 125 instants. The last two rows show the average $\tau_{a\lambda}$ from this work and AERONET respectively.	112
6.6.	Ångström exponents α from this work vs. AERONET (average for the clearest day). Note <i>all</i> corresponds to a linear regression performed with α_i from six wavelengths: 340, 440, 500, 675, 870 nm and also note that AERONET does not have a reported value of α analogous to this, as to be compared.	116
7.1.	Glossary of symbols.	I
7.1.	Glossary of symbols.	II
7.1.	Glossary of symbols.	III
7.2.	Glossary of acronyms.	IV
7.3.	Glossary of Units	V
A.1.	Traceability of spectral irradiance ground measurements.	VIII
A.2.	Traceability of ground measurements: G_h at Salto (LES) and Montevideo (AZT).	VIII
A.3.	Traceability of ground measurements: G_{dh} at Salto (LES).	IX
A.4.	Traceability of ground measurements: G_b at Salto (LES).	IX
B.1.	Air mass coefficients a_i used in REST2 model (Gueymard, 2008b).	XI
B.2.	Typical Aerosol Single Scattering Albedo (ω_g) values by aerosol type, (Hess et al., 1998).	XIII
B.3.	Coefficients a_{ix} used in the SMARTS calculation of air mass, (Eq. 4.2).	XV
B.4.	Vertical profile of atmospheric variables and gases concentrations for STS and STW conditions. From (Gueymard, 1995).	XV
B.5.	Empirical coefficients f_i for different wavelength ranges, for Nitrogen Dioxide transmittance.	XVI
B.6.	α_1 and α_2 empirical values for different relative humidities and different aerosol models.	XVII
B.7.	Coefficients for the Shettle & Fenn aerosol model.	XVIII
C.1.	Minimum, average and maximum values of the atmospheric parameters for each site: Salto (Default, MODIS-AQUA and MERRA-2) and Montevideo (AERONET), during the period of 5 years, from 2020-01-01T00:00 to 2024-12-31T23:59, for 1 minute sampling frequency. The corresponding time series are shown in Fig. C.1.	XXI

C.2. Minimum, average and maximum values of the atmospheric parameters AOD_{550} (adim), w (cm) and u_o (cm), for each data source: Default, AERONET, MODIS-AQUA and MERRA-2. Samples correspond to day 2024-06-18 from 11:15 to 13:41, which is a clear sky, stable atmospheric conditions day. The number of samples is $N = 112$. This table is corresponded with Fig. 4.11.	XXIII
C.3. Minimum, average and maximum values of the atmospheric parameters for each data source: Default, AERONET, MODIS-AQUA and MERRA-2. The number of samples is $N = 2296$ (and 2255), equally distributed into seasons and zenith angles. They have been selected from the period 2020-01-01 to 2024-31-12, where records have originally been taken in 1 minute frequency. Fig. C.2 shows the corresponding time series.	XXIV
C.4. Manufacturer specifications for uncertainty.	XXVI
C.5. Estimated values of uncertainty corresponding to each source.	XXVIII
C.6. SMARTS raw spectral irradiance integrated (280-4000 nm), compared to ground measurements of G_h , G_{dh} and G_b . The table corresponds to day 2024-06-18, with 112 samples selected. The atmospheric parameters used are available in Fig. 4.11, and the corresponding plot is Fig. C.3. MBD and RMSD are shown in absolute (abs, W/m^2) and relative (rel, %) terms.	XXIX

List of Figures

2.1. Irradiance concept and components. Adapted from Wald (2020).	7
2.2. Circumsolar radiation. Note the field of view depends on the measurement instrument. (Figure not to scale). Figure by Paola Russo.	9
2.3. Solar spectrum at TOA (yellow), blackbody approximation (black line) and typical beam solar spectrum at sea level under clear-sky (red). Adapted from: (Rohde, 2008).	10
2.4. Simplified scheme of the absorption and scattering process. Adapted from (Mikuška, 2013).	12
2.5. Particle size of different atmospheric components. Adapted from: (ISO 16890-2:2022, 2022). ePM: efficiency of particulate matter.	12
2.6. Scattering patterns. Adapted from: (Bunge et al., 2006; Wald, 2020)	14
2.7. The absorption of short wave and long wave radiation due to radiatively active gases in the atmosphere happens in different wavelengths. Adapted from (Peixoto and Oort, 1992).	15
2.8. Air mass scheme. Figure by Paola Russo.	16
2.9. Relative air mass parametrizations for several atmospheric components. Figure by Paola Russo.	17
2.10. Plane atmosphere representation for the optical depth, RTE and Lambert Law. Figure by Paola Russo.	18
2.11. Examples of different cloud configurations causing OI. Photographs by Paola Russo.	22
2.12. Satellite view of the sites considered in this work. Source: adapted from Google Earth.	23
2.13. CIMEL sun photometer (extracted from: https://aeronet.gsfc.nasa.gov/new_web/photo_db_v5/Burjassot.html)	24
2.14. Aqua Satellite from NASA https://oceancolor.gsfc.nasa.gov/about/missions/aqua/ , which carries on board the MODIS Spectroradiometer.	26
2.15. Satellite back scattering, adapted from (Danklmayer, 2008) for a passive instrument.	27

2.16. Broadband ground measurements in Salto site, with pyranometers and pyrhelio- meters with fan ventilation, mounted on a sun tracker, which is pointing to the Sun at sunrise (East). Photograph by Paola Russo.	30
2.17. Global spectroradiometer setting for measuring global, diffuse and beam and main components scheme, adapted from EKO (2016). Photograph by Paola Russo. . .	31
2.18. (a) EKO MS711 collimator tube scheme (adapted from EKO (2016)) and (b) the instrument is mounted on its precision solar tracker at Montevideo (photograph by Paola Russo).	32
3.1. Fraction (%) of clear sky samples not tagged as OI versus x_i . Figure by Paola Russo.	38
3.2. Diffuse fraction (f_d) vs clearness index (k_t) diagram for the quality-checked data (shown in grey). The light blue dots indicate clear sky samples and the orange dots identify OI samples. Figure by Paola Russo.	39
3.3. Example of OI detection on a time series (28/01/2020). Figure by Paola Russo. .	40
3.4. Maximum intensity of OIE (W/m^2). Figure by Paola Russo.	41
3.5. OIE duration, Δ (min). The P_{95} duration is 10 minutes. Figure by Paola Russo.	42
3.6. Histograms of Magnitude of OIE, classified by seasons. Energy Magnitude, Mean and P_{95} are expressed in kJ/m^2 . The vertical axis is in logarithmic scale. Figure by Paola Russo.	43
3.7. Histograms of peak intensity (in W/m^2) of OIE, classified by seasons. Figure by Paola Russo.	44
3.8. Over-irradiance occurrences in a solar diagram. Colours indicate the number of occurrences. Figure by Paola Russo.	45
4.1. For different reference atmospheres: (a) effective path-lengths, (b) vertical profiles of relative humidity, atmospheric pressure and temperature. Figure by Paola Russo.	50
4.2. SMARTS transmittances of Ozone (shades of blue) and Nitrogen Dioxide (shades of greens), for several optical path-lengths, $u_{o,i}$ and $u_{n,i}$ (such as 0.01, 1.0 and so on). Adapted from Gueymard (1995).	52
4.3. Water vapour transmittance modelled by SMARTS using $w = 1.419$ cm, the U.S. Standard Atmosphere and $m = 1.5$. Adapted from Gueymard (1995).	54
4.4. Two possible Ångström parametrizations used in SMARTS (Gueymard, 1995). Green: generated using Ångström coefficients $\alpha_2 = 1.3$, $\beta = 0.2$. Blue: generated using $\alpha_1 = 1.3$ (for $\lambda < \lambda_0$, fine particles), $\alpha_2 = 0.8$ (for $\lambda \geq \lambda_0$, coarse particles), $\beta = 0.2$, $\lambda_0 = 675$ nm, $\lambda_1 = 500$ nm. Figure by Paola Russo.	56
4.5. Aerosol transmittance models from (Braslau and Dave, 1973; IAMAP, 1986; Shettle and Fenn, 1979). Modelled with SMARTS (Gueymard, 1995) using STS reference atmosphere, $m = 1.5$, $\tau_{a500} = 0.3442$. Figure by Paola Russo.	57
4.6. Downward angular correction factor for Rayleigh-scattered irradiance, F_R , for different $\tau_{r\lambda}$ values, and different $\cos\theta_z$ angles. Figure by Paola Russo.	59

4.7.	Workflow diagram for SMARTS assessment. Figure by Paola Russo.	67
4.8.	Spectroradiometer EKO MS-711N used for measuring Global Horizontal and Diffuse Horizontal spectral irradiance at ground level (without and with shadow ball mounted respectively). Figure by Paola Russo.	68
4.9.	Shaded-unshaded scheme used for the performance comparisons. The scheme shows the modelled (hat) and observed variables representative of the whole interval but they are actually assigned to the start of their interval, as it is a conventional practice. Spectral dependence is implied in all the variables. The superscript c indicates that variable is obtained using closure (Eq. 2.6). Figure by Paola Russo.	68
4.10.	Time series of the three components of the spectral irradiance integrated in 300-1100 nm: global horizontal (G_h), diffuse horizontal (G_{dh}) and beam normal (G_b), during day 2024/06/18. Figure by Paola Russo.	69
4.11.	Time series of the atmospheric variables of the different data sources: Default, AERONET, MODIS-AQUA, MERRA-2 tested in SMARTS smoothed. Instants correspond to day 2024/06/18 around solar noon. The variables have been interpolated to 1-minute. $\bar{x}$ refers to the mean, and σ is the standard deviation. The maximum, minimum, mean and standard deviation values are shown in (Table C.2). Figure by Paola Russo.	72
4.12.	Sensitivity of SMARTS smoothed to changes in the input parameters: AOD ₅₅₀ , w and u_o , zoomed in the spectral region of main influence of each parameter. The abbreviations correspond to: nom - nominal value tested, high - upper value, low - lower value. The grey spectrum corresponds to irradiance at the top of the atmosphere (Gueymard, 2004) corrected by the sun earth distance correction factor, and it is shown as a reference. Figure by Paola Russo.	76
4.13.	Spectral irradiance vs. wavelength of modelled (SMs+DE, SMs+AE) and observed Global, Diffuse and Beam. Figure by Paola Russo.	78
4.14.	Spectral irradiance vs. wavelength of modelled (SMs+MO, SMs+ME) and observed Global, Diffuse and Beam. Figure by Paola Russo.	79
4.15.	MBD $\pm$ RMSD for the bands 300-400, 400-700, 700-1100 and 300-1100 nm, for every product: Global (Orange), Diffuse (Green) and Beam (Blue), for different composite models: SMs+DE (being the MBD shaped with a circle), SMs+AE (diamond), SMs+MO (star), SMs+ME (square). (In 400-700 nm default and AERONET lines have been moved down for visualization purposes). The dotted lines are axis origins ($0 \text{ W/m}^2\mu\text{m}$) for each spectral range, and the marks in the x axis denote minus and plus $50 \text{ W/m}^2\mu\text{m}$. Figure by Paola Russo.	80
4.16.	Spectral differences between model and measurements. The line represents the mean, while the shaded band shows the maximum and minimum differences during the period analyzed. Figure by Paola Russo.	81

4.17. Scatter plots comparing SMARTS spectral irradiance integrated (300-1100 nm) with EKO measurements of Global ($G_{h,\lambda}$), Diffuse ($G_{dh,\lambda}$) and Direct ($G_{b,\lambda}$) integrated in the same spectral range. See Fig. 4.11 and Table 4.10 for details on the input parameters and performance metrics, respectively. Note that different scales are used for the different variables. Figure by Paola Russo.	84
4.18. Scatter plots of SMARTS (integrated in 280-4000 nm) vs. broadband measurements. Plotted 2249 instants, selected from the period 2020/01/01 to 2024/12/31, originally from 1 minute samples during clear-sky and stable atmospheric conditions. Samples include 28 days equally distributed between seasons and zenith angles. The corresponding performance values are presented in Table 4.10. Figure by Paola Russo.	86
4.19. Broadband performance of the composite model variants (horizontal axis) for G_h (orange), G_{dh} (green) and G_b (blue). The corresponding numeric values are shown in Table 4.12. Figure by Paola Russo.	87
5.1. Atmospheric variables interpolated to 1 minute frequency, for the period considered, 2017-2020. Figure by Paola Russo.	96
5.2. Diffuse fraction vs. clearness index (f_d-k_t) diagram, ground quality checked measurements (blue dots) and clear-sky selection (orange dots). Figure by Paola Russo.	98
5.3. Model performance compared to ground measurements for G_h , G_{dh} , G_b and $G_{h,PAR}$. Figure by Paola Russo.	100
5.4. Model performance for G_h , G_{dh} , G_b and $G_{h,PAR}$ for different $\cos\theta_z$. Figure by Paola Russo.	101
6.1. Methodology scheme. Figure by Paola Russo.	104
6.2. Example of measured spectral irradiance. Measurements taken at Montevideo. Figure by Paola Russo.	105
6.3. Selection of clear-sky instants for two sample days (November 1 and 2, 2022). The x-axis shows the time labels in local time (UTC-3). Figure by Paola Russo.	106
6.4. Estimated circumsolar ratio, CR (expressed as %), for an EKO MS-711 spectroradiometer, depending on the $\tau_{a\lambda}$ level, extracted from García-Cabrera et al. (2020). Figure by Paola Russo.	109
6.5. Langley plots at wavelengths = 340 and 500 nm, for one sample period. The least squares fit to the samples is shown as a red dashed line. Figure by Paola Russo.	110
6.6. U_{95} criteria (WMO/GAW (2004), (Eq. 6.14)) applied at every wavelength, to determine if the values of $G_{s,\lambda}$ estimated return $\tau_{a\lambda}$ that fall within the U_{95} limits: $\pm(0.005 + 0.010/m_a)$, during the instants used for calibration. Figure by Paola Russo.	111
6.7. Results of MBD and RMSD for the whole period and for the clearest day. The error bars are $\pm$ RMSD (unitless). Figure by Paola Russo.	113

6.8.	$\tau_{a\lambda}$ retrieved vs. $\tau_{a\lambda}^0$ AERONET, scatter plots with density information. Figure by Paola Russo.	114
6.9.	Application of the Ångström Law to find parameters α and β through linear regression, using the following wavelengths: (a) the pair $\lambda = 340-440$ nm, (b) the pair $\lambda = 440-870$ nm, (c) six wavelengths, $\lambda = 340, 380, 440, 500, 675$ and 870 nm. The dots indicate the average of $\ln[\tau_{ai}(\lambda)]$ and the vertical grey lines correspond to the minimum and maximum values of $\ln[\tau_{ai}(\lambda)]$. The day used is 2022/Nov/02, from which 125 clear sky instants have been selected. The information is related to Table 6.6. Figure by Paola Russo.	116
A.1.	Grating spectroradiometer parts and functioning principle. Adapted from Edmund Optics (2024).	VII
C.1.	Time series of atmospheric parameters from different data sources, during the period 2020-01-01 00:00 to 2024-12-31 23:59, at 1 minute frequency, for the sites Montevideo (AERONET) and Salto (MODIS/AQUA and MERRA-2). Corresponding statistics in Table C.1. Figure by Paola Russo.	XXII
C.2.	Time series of the atmospheric parameters during the selected instants to analyse SMARTS broadband. Period 2020-01-01 00:00 to 2024-12-31 23:59, at 1 minute frequency, for the sites Montevideo (source: AERONET) and Salto (sources: MODIS/AQUA and MERRA-2). Corresponding statistics in Table C.3. Figure by Paola Russo.	XXV
C.3.	Scatter plots of SMARTS raw spectral irradiance integrated (280-4000 nm), compared to ground measurements of G_h , G_{dh} and G_b . The plot corresponds to day 2024-06-18, with 112 samples selected. The atmospheric parameters used are available in Fig. 4.11 and the corresponding performance metrics are available at Table C.6. Figure by Paola Russo.	XXX