

# OTSun: An Open Source Code for Optical Analysis of Solar Thermal Collectors and PV Cells

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## Abstract

The OTSun project is a research project whose main objective is to develop an open-source software to simulate the optical behavior of solar collectors. In this Monte Carlo ray tracing program, the trajectory of light rays is determined by the Fresnel equations of electromagnetic optics. The geometry of the solar collector is generated using the free software FreeCAD, allowing the user to visualize the scene. OTSun determines the optical efficiency of solar thermal collectors and photovoltaic solar cells. Its library is hosted on GitHub and, to make it more user-friendly, a webtool has been developed. This paper describes the implemented algorithm as well as the types of materials available in the library. Two simple cases are presented, step by step, to allow for a correct simulation of solar thermal collectors and photovoltaic solar cells.

*Keywords:* ray-tracing, open-source, solar energy collector, solar cells

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## 1. Introduction

The OTSun project is a research project financed by the Spanish Ministry of Economics and Competitiveness (MINECO) as well as the European Regional Development Fund (ERDF) (ENE2015-68339-R). The main objective is to develop an open-source software for the optical analysis of solar collectors (Pujol-Nadal et al., 2016.). The duration of the project is from 2016 to 2019. Physical equations that best describe the interaction between radiation and material were implemented to provide high precision results for optical simulations. These equations include the dependency on the wavelength, the polarization, and the incidence angle of the electromagnetic (EM) wave. The algorithm is based on the Monte Carlo ray tracing (MCRT) principle. Interference phenomena can also be taken into account for simulations by means of a pre-processing step using the transfer-matrix method (TMM). OTSun uses the open-source program FreeCAD as a graphical user interface, which allows the user to design and import the geometry of a collector in a user-friendly manner. The simulations further allow the user to determine the optical efficiency of both solar thermal collectors and photovoltaics.

### 1.1. Graphical user interface: FreeCAD

OTSun uses FreeCAD to model and visualize 3D objects of a scene. Since FreeCAD is an open-source code, the OTSun project can benefit directly from the contributions of programmers and users from all over the world. However, this also means that in order to begin a simulation with OTSun, it is crucial to have the collector geometry available in the FreeCAD-specific file format \*.FCStd. In this geometry file, the optical properties are assigned to the different collector components that interact with the EM wave. The different components, in turn, consist of either surface or volume elements. Once the geometry is imported, the sun window is created, which is the region from where the rays are emitted. The sun window is rectangular in shape and its size is automatically adjusted to the collector dimensions to save CPU time.

### 1.2. The optical model

The algorithm is based on an MCRT approach. Starting at the sun window, the trajectory of the rays is determined by the Fresnel equations for EM waves, taking into account wavelength, polarization, and incidence angle. The reflectance coefficient  $R$  and the transmittance coefficient  $T = 1 - R$  are given by Eqs. (1)-(2) (Macleod, 2010):

$$R = \left( \frac{\eta_1 - \eta_2}{\eta_1 + \eta_2} \right) \left( \frac{\eta_1 - \eta_2}{\eta_1 + \eta_2} \right)^* \quad (1)$$

$$\eta_i = \begin{cases} \frac{N_i \cos \vartheta_i}{Z_0}, & s - \text{polarized} \\ \frac{N_i}{Z_0 \cos \vartheta_i}, & p - \text{polarized} \end{cases} \quad (2)$$

where  $Z_0 = \sqrt{\frac{\mu_0}{\epsilon_0}}$  is the optical impedance of free space and  $N(\lambda) = n(\lambda) - ik(\lambda)$  the complex refractive index.

The real part is the refractive index and the imaginary part represents the extinction coefficient. The complex refractive angle  $\vartheta_i$  can be calculated by means of Snell's law, Eq. (3).

$$N_1 \sin \vartheta_1 = N_2 \sin \vartheta_2 \quad (3)$$

When a ray is refracted and passes through to the interior of a transparent material with an extinction coefficient, the energy of the ray is attenuated according to the Beer-Lambert law, Eq. (4).

$$E(x, \lambda) = E_0(0, \lambda) e^{-\alpha(\lambda)x} \quad (4)$$

where  $\alpha(\lambda) = 4\pi k(\lambda)/\lambda$  is the absorption coefficient.

### 1.3. The OTSun webtool

The OTSun code, implemented in Python, is available on GitHub (Cardona and Pujol-Nadal, 2018). As the direct use of the OTSun library requires some Python programming skills, a webtool helps the user navigate through the simulation and easily input parameters. The user can choose from three different simulations, all of which take into account the Buie sun model (Buie et al., 2003).

- *Single experiment with plot of rays*: This simulation visualizes the scene. It produces a \*.FCStd file that contains the collector geometry together with the trajectories of the emitted rays for a single sun position.
- *Spectral analysis*: This simulation obtains the optical efficiency for a single sun position with a user-defined range of wavelengths. The result are different \*.txt files that contain the spectral efficiency.
- *Total analysis*: This simulation obtains the optical efficiency for different sun positions using the standard model for direct solar radiation ASTM G173. The result is stored in \*.txt files.

The webtool can be accessed via <http://otsun.uib.es/otsunwebapp/node/start>. Fig. 1 shows a flow chart of the different tasks. The first step is to provide an email address for delivery of the results. The second step is to upload the \*.FCStd file, which contains the geometry of the solar collector. In the third step, the material properties are specified. If all the material files are available, they can simply be uploaded together as a \*.zip file. If this is not

the case, a hyperlink redirects the user to the Creator of Materials page, where the OTSUn-specific material files can be defined manually. The next step is to specify the type of simulation under Experiment to Run. The last step is to define the ray-tracing input parameters under Input Parameters. Once the simulation is running, the app redirects the user to a webpage where the progress is displayed.

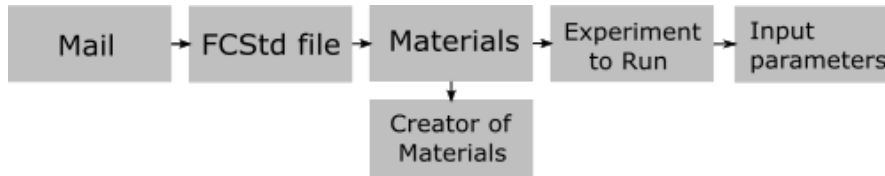


Fig. 1 Flowchart of the different stages of an OTSUn webtool simulation.

## 2. Material types

When a ray is incident on a surface, it will be either reflected or transmitted depending on the Fresnel coefficients  $R_{s/p}(\theta, \lambda)$  and  $T_{s/p}(\theta, \lambda)$  (Eqs (1)-(2)) of the material. Both coefficients, which originate from the complex refractive index of the material, depend on the wavelength, the incidence angle  $\theta$ , and the polarization of the incident light (polarization  $s/p$ ). OTSUn distinguishes between two types of materials: volume and surface materials. For more details on the nomenclature and mathematical expressions, see (Hertel et al., 2016)

### 2.1. Volume material

- *Constant Refractive Index*: Material with a constant refraction index and absorption coefficient given by  $n$  and  $\alpha$ . The absorption, which occurs in the material (Eq. (4)), leads to a loss of energy.
- *Variable Refractive Index*: Material with a refraction index that depends on the wavelength. It is necessary to provide the \*.txt file that contains the following columns:  $\lambda$  (nm),  $n$ , and  $k$ . The absorption, which occurs in the material (Eq. (4)), leads to a loss of energy.
- *PV Material*: Material used to simulate active materials in photovoltaic cells. This material has the same characteristics as the Variable Refractive Index, with the exception that the absorption in the material is the useful energy, which gives rise to the creation of electron/holes pairs and therefore conversion to electric energy.
- *Thin-Film Material*: Material whose coefficients  $R_{s/p}(\theta, \lambda)$  and  $T_{s/p}(\theta, \lambda)$  are previously calculated using the TMM. It is necessary to provide a \*.txt file with the following columns:  $\lambda$  (nm),  $\theta$  (deg),  $R_s$ ,  $R_p$ ,  $T_s$ , and  $T_p$ . Furthermore, the materials in contact with the TMM layer should be indicated (upper and lower surface). The refraction indices can be provided as a \*.txt file, as with the Variable Refractive Index.

### 2.2. Surface material

- *Opaque Simple Layer*: Material with total absorption and without any contribution to useful energy gain.
- *Transparent Simple Layer*: Material with a constant transmittance  $T$  and without absorption.
- *Absorber Simple Layer*: Material with constant absorption  $\alpha$  and  $T = 0$ . The absorbed rays contribute to the useful energy gain of the solar thermal collector.
- *Absorber Lambertian Layer*: Material with constant absorption  $\alpha$ , Lambertian (total diffuse) reflection, and  $T = 0$ . The absorbed rays contribute to the useful energy gain of the solar thermal collector.
- *Absorber TW Model Layer*: Material with  $\alpha$  for normal incidence, together with  $b$  and  $c$  constants, which describe the incidence angle dependency of the model of (Tsfamichael and Wäckelgård, 2000). Reflection is Lambertian. Transmittance is  $T = 0$ . The absorbed rays contribute to the useful energy gain of the solar thermal collector.
- *Absorber Polarized Coating Layer*: Material with  $T = 0$ , where absorption  $\alpha$  depends on the wavelength and incidence angle. A \*.txt file should be provided with the following columns:  $\lambda$  (nm),  $\theta$  (deg),  $R_s$ , and  $R_p$ .

- *Reflector Specular Layer*: Material with specular reflection, constant  $R$ , and  $T = 0$ . It is also possible to define Gaussian or bi-Gaussian scattering (Pettit, 1977) with the parameters  $\sigma_1$  (mrad),  $\sigma_2$  (mrad), and the weighting factor  $k_{\sigma_1}$  for the Gaussian curve with variance  $\sigma_1$ .
- *Reflector Lambertian Layer*: Material with Lambertian reflection, constant parameter  $R$ , and  $T = 0$ .
- *Reflector Specular Metallic Layer*: Metallic, specular material with a complex refractive index  $N(\lambda)$ . The refractive index should be provided as a \*.txt file with the following columns:  $\lambda$  (nm),  $n$ , and  $k$ . Gaussian or bi-Gaussian scattering can be defined the same as for the reflector specular layer. The reflectance will be calculated based on the Fresnel equations (1)-(2).
- *Reflector Polarized Coating Layer*: Material with  $T = 0$  and  $R$  provided as a \*.txt file with the following columns:  $\lambda$  (nm),  $\theta$  (deg),  $R_s$ , and  $R_p$ . Scattering can be defined in the same manner as in the reflector specular layer.
- *Create Material From Two Layers*: Surface material where different properties can be assigned to each side. The user can chose from any of the previously described surface models.

### 3. Simulation of a parabolic trough collector

This section describes how to conduct a simulation of a parabolic trough collector (PTC). The PTC under consideration consists of three basic elements: the parabolically shaped mirror, the absorber tube, and the glass envelope with anti-reflectance layer. The optical properties of the anti-reflectance layer, which is a thin layer where interference effects occur, have been calculated by means of a TMM algorithm (Steven Byrnes, 2018.). The tests folder on <https://github.com/bielcardona/OTSun> contains all files required for this simulation. One of these files is test\_PTC.FCStd, which contains the geometry of the collector seen in Fig. 2. The figure also shows the different components of the collector with their respective optical property labels in parentheses.

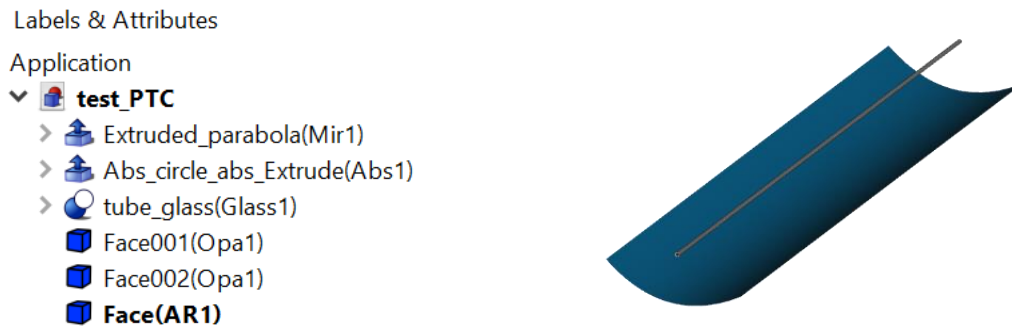


Fig. 2 Screenshot from the FreeCAD file test\_PTC.FCStd. The optical property labels are clearly visible in parentheses.

After accessing the webtool, the user types in an email address and uploads the file test\_PTC.FCStd. The next webpage, Materials, displays a list of all optical property labels that have been detected in the geometry file and are now expected to be provided by the user (Fig. 3).

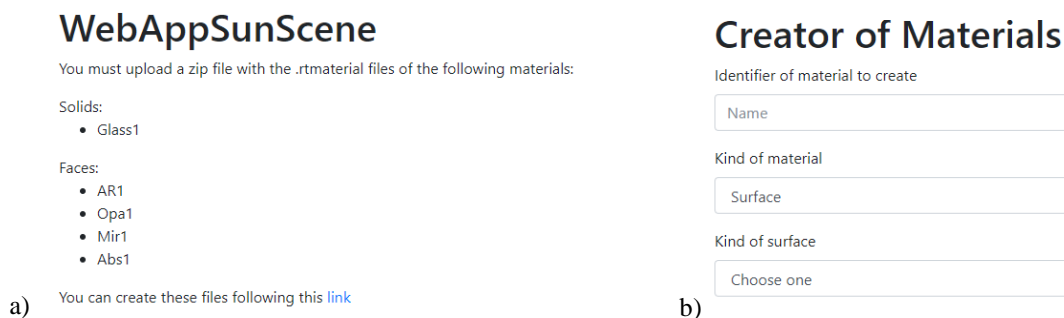


Fig. 3 a) The labels of the optical properties defined in the \*.FCStd file. b) Template to define optical properties.

To create material files manually, the user is redirected to the Creator of Materials webpage via the hyperlink <http://otsun.uib.es/otsunwebapp/material>. First, the user enters the material names, which must be identical to the

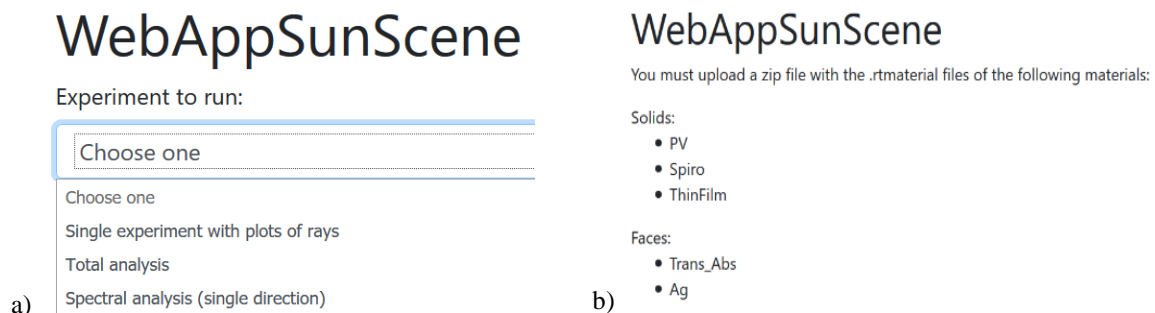
optical property labels specified in the \*.FCStd file in parenthesis. In the next step, the user specifies the material type, either surface or volume. As detailed in the previous chapter, the user provides all the different optical models and their respective parameters in the remaining fields. In this example, the materials are defined according to Table 1.

The webtool saves each material as an app-specific binary file \*.otmaterial. Once all the material files have been created, they should be uploaded together in a zip folder. After defining the materials, the user chooses the desired simulation under Experiment to Run (Fig. 4). In this example, a total analysis was selected, which requires the following parameters: sun position ( $\phi = 0$ ,  $\theta = 0$ ), number of rays for each sun position (100000), PTC aperture area (19090215 mm<sup>2</sup>), and creation of ray instances according to the Buie model ( $CSR=0.05$ ).

The results are sent to the provided email address, and they can also be accessed via the hyperlink on the last page of the webtool. In this example, the result is an optical efficiency of 82.5%.

**Table 1** Material types generated for the PTC.

Name	Type of material	Source
Glass1	Volume – Variable Refractive Index	BK7_Schott.txt
AR1	Surface – Transparent Polarized Coating Layer	AR-J.txt: MgF2 (Hertel et al., 2018)
Mir1	Surface – Reflector Specular Layer	R = 0.94
Abs1	Surface – Absorber Simple Layer	$\alpha = 0.95$
Opal	Surface – Opaque Simple Layer	



**Fig. 4** a) Screenshot of the different simulations available. b) Materials which have been defined for the solar perovskite cell.

#### 4. Simulation of a photovoltaic cell

This section explains the steps for conducting a simulation of a 200 nm perovskite photovoltaic cell. As with the PTC simulation, all files for this simulation can be found in the test folder on GitHub. This simulation is analogous to the PTC simulation, except the geometry is defined by Perovskite\_Stack\_200nm.FCStd. Examples of the different materials, which are specified in the \*.FCStd file, are shown in Fig. 5. The configuration of the solar cell is shown in Fig. 5a and the different optical parameters are summarized in Table 2. The material thin film is an assembly of four layers that are in contact with the perovskite substrate. The optical properties of this multi-layer assembly were calculated using the TMM algorithm.

Table 2 Geometry and material type available for solar cell simulations.

Name	Type of material	Source
Thin_Film	Volume – Thin Film Material	Fitxer_OTSun_Exp1a_theta0_90.txt
PV	Volume – PV Material	Perovskite_Leguy.txt
Spiro	Volume – Variable Refractive Index	Spiro_.txt
Ag	Surface – Reflector Specular Layer	Ag_Yang.txt

For this example, a spectral analysis (single direction) was conducted at normal incidence, with 1000 rays per wavelength in the range of 300 to 900 nm, and a step size of 2 nm. The aperture area of the photovoltaic collector is  $10^6 \text{ mm}^2$ . As with the previously discussed PTC simulation, the results are sent by email:

- *PV\_spectral\_efficiency.txt*: Spectral optical efficiency of the photovoltaic material (absorbed energy that generates electron/holes pairs)
- *PV\_paths\_values.txt*: Information about the ray trajectories inside the PV material
- *source\_wavelengths.txt*: Information about the light source

Fig. 5b shows the spectral optical efficiency obtained by OTSun compared to the one obtained by the TMM algorithm. Since both curves are similar, the OTSun code is validated.

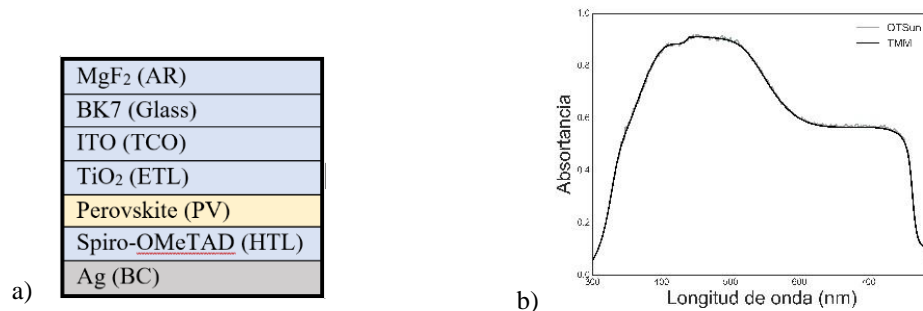


Fig. 5 a) Thin-film assembly of the perovskite cell. b) Spectral, optical efficiency obtained by OTSun and the TMM algorithm respectively.

## 5. Conclusions

This study described the OTSun webtool for optical simulations, including the underlying mathematical principles of radiation-material interaction and the variety of materials available for testing. A step-by-step approach of how to use the OTSun webtool was presented using the examples of a PTC collector and a perovskite solar cell.

## 6. Acknowledgment

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