# SOLEY User Manual Version 1.0.0

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## Contents

# 1 Introduction

## 1.1 Purpose and Scope of SOLEY

SOLEY (Solar Cell Optics and Electrics) is a simulation package designed for researchers, engineers, and students working with photovoltaic devices. Its primary purpose is to provide an efficient and accessible platform for modelling the optical and electrical performance of single-junction and multijunction solar cells. The software bridges the gap between complex drift-diffusion solvers and simpler analytical models, and it aims to offer a balance of accuracy, speed, and ease of use. SOLEY is intended for simulating planar, multilayer solar cell structures and predicting key performance metrics like $J_{sc}$, $V_{oc}$, Fill Factor (FF), and efficiency ($\eta$).

## 1.2 Key Features and Capabilities

SOLEY offers a range of features for comprehensive solar cell analysis:

- **Optical Simulation:** Utilises the Transfer Matrix Method (TMM) to calculate reflectance, transmittance, absorbance, and optical generation profiles within the device stack. Supports both direct and diffuse illumination.
- **Electrical Device Modelling:** Employs a detailed balance framework incorporating radiative, Auger, and Shockley-Read-Hall (SRH) recombination mechanisms to determine $J$-$V$ characteristics and performance parameters. Allows for detailed defect analysis via the SRH module which is designed to accommodate both experimentalists and theoreticians.

- **Layer Mixing:** Includes the Bruggeman Effective Medium Approximation (EMA) to simulate layers composed of mixed materials.
- **Optimisation:** Features a tool for optimising the thickness of selected layers to maximise device efficiency based on a grid search algorithm.
- **Batch Processing:** Enables automated parameter sweeps for efficient exploration of the device design space. Users can vary general parameters (like temperature) or absorber-specific parameters (like resistances or recombination coefficients).

## 1.3 Underlying Physical Models (Brief Overview)

SOLEY's calculations are based on established physical models:

- **Optics:** The Transfer Matrix Method (TMM) calculates how light propagates through and is absorbed by the different layers of the solar cell.
- **Electronics:** A detailed balance model, extending the Shockley-Queisser limit, is used. It considers the generation of carriers from absorbed light and their loss through various recombination pathways (radiative, Auger, SRH). The model incorporates the effects of series and shunt resistance. For multijunction cells, current matching between subcells is enforced for 2-terminal configurations.

These models allow for rapid yet physically meaningful simulations of device behaviour. A more detailed theoretical background is provided in Section 4.

## 1.4 Existing Solar Cell Modelling Software

Numerous software tools have been developed to simulate and analyse photovoltaic (PV) devices, each adopting different theoretical and numerical approaches. Widely adopted tools include SCAPS, SolCore, AFORS-HET, WX-AMPS, OghmaNano, Sentaurus, and Silvaco.

These programs typically employ advanced drift-diffusion models coupled with Poisson's equation and carrier continuity equations. Specifically, drift-diffusion modelling involves solving the coupled semiconductor equations:

$$\text{Poisson equation:} \quad \nabla \cdot (\epsilon \nabla \psi) = -q(p - n + N_D^+ - N_A^-) \tag{1}$$

$$\text{Electron continuity:} \quad \frac{1}{q}\nabla \cdot J_n = G - R_n - \frac{\partial n}{\partial t} \tag{2}$$

$$\text{Hole continuity:} \quad -\frac{1}{q}\nabla \cdot J_p = G - R_p - \frac{\partial p}{\partial t} \tag{3}$$

$$\text{Electron drift-diffusion current:} \quad J_n = q\mu_n nE + qD_n \nabla n \tag{4}$$

$$\text{Hole continuity current:} \quad J_p = q\mu_p pE - qD_p \nabla p \tag{5}$$

where $J_n$ and $J_p$ are electron and hole current densities, $G$ and $R$ represent generation and recombination rates, $N_D^+$ and $N_A^-$ are ionised donor and acceptor concentrations, and $\mu_n$, $\mu_p$, $D_n$, and $D_p$ are carrier mobilities and diffusivities. Solving these coupled differential equations allows detailed modelling of carrier transport and recombination in semiconductor devices. The contribution of those packages for advancing the community's

understanding of solar cells cannot be overstated, and researchers in the field of PV are strongly encouraged to integrate one of those in their workflow.

**Strengths of existing software**:

- High fidelity modelling of semiconductor physics through the drift-diffusion approach.
- Inclusion of comprehensive recombination mechanisms (Shockley-Read-Hall, radiative, Auger) and detailed material properties.
- Capability to generate detailed electrical characteristics such as band diagrams, electric fields, and carrier profiles.
- Established validation through extensive literature use.

Hence, making a meaningful contribution in this landscape is challenging. After having used SCAPS extensively over the years, dating back to my days as a PhD student, and having occasionally played with some of the aforementioned software, I identified specific points which could be addressed by a new package:

- Steep learning curve, requiring considerable training and experience.
- Complex input parameter definitions, often requiring detailed knowledge of material properties for all layers in the stack.
- High computational costs for complex structures, limiting rapid iteration.
- Difficulties with transparency and reproducibility of results due to intricate numerical configurations.

Given these considerations, there could be a need within the PV research community for a complementary tool that balances accuracy, transparency, ease of use, and accessibility, motivating the development of SOLEY.

## 1.5 Justification for SOLEY

Existing solar cell simulation tools provide highly detailed modelling approaches but often suffer from complexity, computational intensity, and a steep learning curve. **SOLEY** has been developed to provide a powerful, accurate, and flexible framework for photovoltaic device modelling that retains computational efficiency while maintaining predictive accuracy.

Unlike many traditional simulation tools that require highly detailed input parameters and mesh-dependent numerical solvers, **SOLEY** adapts to the level of available information. It allows users to perform accurate device modelling whether they rely on experimentally extracted parameters from fitting or theoretical predictions from first-principles calculations.

### 1.5.1 High Accuracy and Predictive Power

Despite its flexibility, **SOLEY** retains high predictive accuracy by incorporating fundamental physical models that govern photovoltaic operation:

- **Optical Modelling:** Uses the *Transfer Matrix Method* (TMM) to precisely compute reflectance, absorbance, and transmittance in multilayer structures, ensuring accurate determination of light absorption profiles in complex architectures.
- **Charge Transport and Recombination:** Implements a *detailed balance framework* while incorporating realistic recombination mechanisms, including Shockley-Read-Hall (SRH), Auger, and radiative recombination. This enables calculation of realistic open-circuit voltage, fill factor, and efficiency.
- **Numerical Stability:** Employs computational techniques to prevent divergence of the TMM, ensuring energy conservation and physically meaningful results in a braod range of configurations (yes, it can still be broken if one tries hard enough).

### 1.5.2 Versatility and Adaptability

One of SOLEY's key strengths is its ability to seamlessly adapt to different levels of input complexity:

- **Experimentalists:** Can directly use extracted parameters (e.g., recombination currents, defect densities, optical constants) from real devices to analyse performance and guide further optimisation.
- **DFT and First-Principles Modellers:** Can incorporate parameters derived from first-principles calculations to predict solar cell performance before experimental realisation.
- **Users with Limited Data:** When detailed parameters are unavailable, SOLEY provides physically reasonable estimates to enable meaningful analysis, allowing users to progressively refine their models as more data become available.

This flexibility ensures that SOLEY is not only a tool for rapid evaluation but can also be viewed as a comprehensive modelling package for more rigorous photovoltaic research.

### 1.5.3 Target Audience: A Tool for Experimentalists and Theorists

**SOLEY** is designed to be accessible to a broad spectrum of researchers, providing modelling capabilities with well-reported equations without the complexity of traditional drift-diffusion solvers:

- **Experimental researchers:** Enables precise interpretation of photovoltaic performance using extracted material parameters and device-specific measurements.
- **Density Functional Theory (DFT) and semiconductor theorists:** Allows direct integration of computationally derived parameters to predict device efficiency and behaviour.
- **Educators and students:** Serves as an intuitive platform to explore photovoltaic concepts with real-world physical modelling.

### 1.5.4 A Powerful Complement to Traditional Tools

Rather than being a simplified version of existing tools, **SOLEY** is a powerful complement that excels in:

- **Accurate Performance Prediction:** Provides results comparable to drift-diffusion solvers when applied within its methodological framework.
- **High Computational Efficiency:** Avoids the overhead of finite-element meshing while delivering detailed device insights.
- **Broad Applicability:** Supports single-junction, tandem, and multijunction devices with up to six absorbers, making it suitable for state-of-the-art solar cell architectures.

By combining **scientific rigour, computational efficiency, and user flexibility**, SOLEY represents an unusual approach to solar cell modelling that can serve both the experimental and theoretical researchers.

## 1.6 Philosophy of SOLEY

While SOLEY does have obvious limitations, like any tool, SOLEY is built on a physics-driven, parameter-flexible approach that allows both high-precision modelling and quick exploratory analyses.

This section defines the **core principles** of SOLEY, its **scope**, and what it **does not aim to do**.

### 1.6.1 Core Principles of SOLEY

SOLEY is developed around three key principles:

- **Scientific Rigour:** The software implements physically sound models from fundamental semiconductor and optical physics. Every calculation follows well-established theories, ensuring results that are accurate and interpretable.
- **Computational Efficiency:** While maintaining accuracy, SOLEY avoids a lot of the computational complexity. The software is designed to deliver results quickly.
- **Flexibility and Accessibility:** SOLEY use can be adapted to various user needs, whether using detailed experimental parameters, first-principles calculations, or estimated values. This versatility allows researchers from different backgrounds (experimental, theoretical, and maybe even industrial) to use it effectively.

### 1.6.2 Scope of SOLEY

SOLEY is designed to model **the fundamental optoelectronic processes** in photovoltaic devices, allowing researchers to explore a wide range of solar cell architectures. The software covers:

- **Optical Modelling:** Computes absorption, reflectance, and transmittance using the *Transfer Matrix Method* (TMM), ensuring precise calculation of light propagation and interaction in multilayer structures.

- **Charge Transport and Recombination:** Implements a **detailed balance approach** that captures key recombination mechanisms: Shockley-Read-Hall (SRH), Auger, and radiative recombination. This allows accurate computation of current-voltage ($J$-$V$) characteristics.
- **Multijunction Solar Cells:** Supports the modelling of **tandem and multi-junction solar cells with up to six absorbers**, incorporating current-matching techniques and an accurate fill factor estimation for 2T configuration.
- **Defect-Driven Device Analysis:** Provides a detailed recombination parameterisation framework, allowing users to explore the effects of bulk and interface defects through realistic Shockley-Read-Hall (SRH) modelling. The equation used are given later in this manual.
- **Energy-Loss Mechanisms and Optimisation:** Quantifies power losses due to Auger recombination, series/shunt resistances, and thermalisation, helping researchers optimise device structures efficiently.

### 1.6.3 What SOLEY Does Not Aim to Do

It is important to clarify the methodological boundaries of SOLEY. The software does not aim to:

- **Perform Drift-Diffusion Simulations:** Unlike, SCAPS, AFORS-HET, or AMPS, SOLEY does not solve the full set of semiconductor transport equations, such as the Poisson and drift-diffusion equations. Instead, it focuses on a **detailed balance and recombination-based approach**, which is more computationally efficient while retaining high accuracy. It also means a more limited amount of outputs: basically, SOLEY will output a JV curve and an optical profile, but things such as C-V-T etc are beyond the capabilities of SOLEY.
- **Simulate Full Electromagnetic Wave Propagation:** SOLEY employs the Transfer Matrix Method (TMM) for optical modelling rather than finite-difference time-domain (FDTD) or rigorous coupled-wave analysis (RCWA). This provides excellent accuracy for multilayer structures while remaining computationally efficient. However, it also has inherent limitations in terms of layer thickness, for example.
- **Compute Band Diagrams:** SOLEY does not explicitly solve for the electronic band structure of materials. Instead, it allows users to input precomputed bandgap values, effective masses, and recombination parameters from experimental measurements or first-principles calculations.

# 2 Getting Started: A Basic Simulation Workflow

This section guides you through a typical simulation process in SOLEY.

## 2.1 Launching the SOLEY Application

The main window will appear directly when opening the software.

## 2.2 Building a Simple Device Stack

The device structure is defined as a stack of layers.

- Click the **Add Layer** button. Remember, the first and last layer of the stack should always be the ambient medium (Air in most cases).
- A file dialog opens. Select the text file containing the optical constants (n, k values vs. wavelength) for your first layer. These files should be located in an accessible folder, typically named `Optical_Indices`. You can use comments but the formatting should be with ascending wavelength in nm.
- An input box appears. Enter the thickness of this layer in nanometres (nm).
- The layer appears in the **Layer List Panel** on the top left.
- Repeat this process to add all layers in your device stack, from the layer where light enters first (top) to the substrate or back contact (bottom).

## 2.3 Defining Layer Properties

In the **Layer List Panel**:

- Adjust the **thickness** of any layer by editing the value in its corresponding entry box.
- Use the **Up** and **Down** buttons to reorder layers.
- Use the **Remove** button to delete a layer.

## 2.4 Setting Basic Calculation Parameters

In the **Calculation Parameters** panel (bottom left):

- Define the **Wavelength Range** (Min, Max) and **Step** in nm for the optical simulation.
- Set the **Incidence Angle** in degrees (0 for normal incidence).
- Choose the light **Polarisation** (TE, TM, or Unpolarised).

## 2.5 Running the Optical Calculation

Click the **Run Optical Calculation** button located below the Calculation Parameters. SOLEY calculates the optical properties based on the defined stack and parameters. The calculation may take a few seconds depending on the complexity and wavelength range. Takes longer with diffuse light.

## 2.6 Interpreting the Optical Results Plot

The main plot area (top right) displays the results:

- **Reflectance (R):** Fraction of light reflected from the device (Red line).
- **Transmittance (T):** Fraction of light passing through the entire stack (Blue line).
- **Absorbance (A):** If 'Calc A' is checked for specific layers, their absorbance is plotted (Other colours). Total absorbance (A) and the sum R+T+A (which should ideally be 1) are also shown. The plot can quickly get crowded, so I recommend just exporting the data.

## 2.7 Defining Absorber Layers and Bandgaps

To perform electrical calculations, define which layers act as absorbers:

- In the **Layer List Panel**, check the **Absorber** box for each layer that should absorb light and generate carriers.
- The bandgap is not automatically calculated (e.g., from absorbance profile) but often wrong, so enter the bandgap value (in eV) in the corresponding **Bandgap** entry box within the **Device Modelling Panel** (bottom right). Up to six absorbers can be defined.
- Click the **Update Bandgap** button below the entry boxes if you entered values manually. Don't forget, seriously.

## 2.8 Setting Basic Device Parameters

In the **Device Modelling Panel** (bottom right):

- Select the incident light **Spectrum File** (e.g., AM1.5G most of the time).
- Set the device operating **Temperature** (K) which is 300K by default. There used to be an input box for the Étendue too, but I removed it as no one seems to need it. However, Étendue is still available as a batch parameter if you are that kind of person.
- Input **Series (Rs)** and **Shunt (Rsh)** resistances (in Ohm·cm$^2$) for each defined absorber layer. Same for the Auger coefficients.

Other parameters like injection factor, and SRH parameters can be set for more detailed modelling (see Section 6).

## 2.9 Running the Device Calculation

Click the **Calculate Device Parameters** button. SOLEY uses the optical calculation results and the device parameters to compute the electrical performance.

## 2.10 Interpreting the Device Results Table

The results appear in the table at the bottom of the Device Modelling Panel:

- Each row corresponds to an absorber layer.
- Columns show key metrics: Bandgap (eV), $V_{oc}$ (V), $J_{sc}$ (mA/cm$^2$), FF (%), Efficiency (%), and various loss components (those can be sometimes buggy, will be addressed in a future update).
- If multiple absorbers are defined, a final row shows the calculated performance for the 2-terminal multijunction device (current-limited).

## 2.11 Saving the Simulation

To save the current device stack and all parameters:

- Click the **Save Simulation** button.
- Choose a file name and location. The simulation state is saved as a `.soley` file (JSON format).
- Use the **Load Simulation** button to open previously saved files. If you moved the optical sepctrum files, it is not going to work.

# 3 Graphical User Interface (GUI) Overview

This section describes the main components of the SOLEY user interface.

## 3.1 Main Window Layout

The main window is divided into four primary areas (quadrants):

- **Top Left:** Layer List Panel - Defines the device structure.
- **Bottom Left:** Calculation Parameters and Action Buttons - Controls simulation settings and execution.
- **Top Right:** Plotting Area - Displays optical results (R, T, A).
- **Bottom Right:** Device Modelling Panel - Sets electrical parameters and displays device results.

## 3.2 Layer List Panel (Top Left)

This panel manages the layers of the solar cell stack.

- **Layer Display:** Shows layers from top (light incident side) to bottom. Each layer entry displays its name (from the optical file), thickness, and control widgets.
- **Thickness Entry:** Allows direct editing of layer thickness (nm).

- **Absorber Checkbox (✓):** Marks the layer as an active absorber for electrical calculations.
- **Calculate A Checkbox (✓):** Instructs SOLEY to calculate and plot the absorbance specifically for this layer during the optical simulation.
- **Mix Checkbox (✓):** Enables mixing of this layer with the one immediately below it using the Bruggeman EMA model. Only appears if the layer is not the last one.
- **Mix Ratio Slider:** Appears when 'Mix' is checked. Controls the volume fraction of the current layer in the mixture (0.0 to 1.0).
- **Up/Down Buttons:** Change the layer's position in the stack.
- **Remove Button:** Deletes the layer from the stack.
- **Add Layer Button:** Located below the list, used to add new layers.

## 3.3 Calculation Parameters Panel (Bottom Left)

This panel controls the optical simulation settings.

- **Wavelength Min/Max/Step:** Defines the spectral range and resolution (nm).
- **Incidence Angle:** Angle of incoming light relative to the surface normal (degrees).
- **Polarisation:** Selects Transverse Electric (TE), Transverse Magnetic (TM), or Unpolarised light.
- **Smoothing Controls:**
  - **Enable Smoothing Checkbox (✓):** Activates/deactivates Savitzky-Golay smoothing of the calculated R, T, A data.
  - **Window Length:** Sets the filter window size (odd integer).
  - **Polynomial Order:** Sets the order of the polynomial used for smoothing.
- **Diffuse Light Controls:**
  - **Diffuse Light Checkbox (✓):** Switches calculation mode from direct incidence to diffuse (hemispherical) illumination.
  - **Angle Steps:** Sets the number of discrete angles used to approximate the hemisphere.
- **Run Optical Calculation Button:** Executes the optical simulation with the current settings.

## 3.4 Plotting Area (Top Right)

Displays the results of the optical calculation.

- Shows Reflectance (R), Transmittance (T), and individual layer Absorbance (A) versus wavelength.
- Includes Total Absorbance and the sum R+T+A for verification.
- Plot updates automatically after running the optical calculation.
- Title indicates polarisation and angle used.
- Grid lines aid visualisation.
- A separate window for plotting J-V curves is accessed via the **Plot J-V Curve** button in the Device Modelling Panel.

## 3.5 Device Modelling Panel (Bottom Right)

Controls parameters for the electrical simulation and displays results.

- **Spectrum File Selection:** Browse and select the incident solar spectrum file (`.txt` format).
- **Temperature (K):** Operating temperature of the device.
- **Injection Factor Slider:** Logarithmic slider adjusts the intensity of the incident spectrum (simulates concentration). The label shows the equivalent power density ($mW/cm^2$) or concentration factor.
- **Series & Shunt Resistances:** Input fields for Rs and Rsh ($Ohm \cdot cm^2$) for each defined absorber (up to 6).
- **Auger Coefficients:** Input fields for electron (Cn) and hole (Cp) Auger coefficients ($cm^6/s$) for each defined absorber (up to 6).
- **Bandgap Entries:** Input fields for the bandgap (eV) of each defined absorber layer. Use the **Update Bandgap** button to apply manually entered values.
- **SRH Recombination Frame:** Contains buttons (**Absorber 1** to **Absorber 6**) that open the **Define Defect Profile** window for detailed SRH parameter input (see Section 6.3).
- **Results Table:** Displays calculated device parameters ($V_{oc}$, $J_{sc}$, FF, $\eta$, losses) for each absorber and the overall multijunction device.
- **Calculate Device Parameters Button:** Executes the electrical simulation.
- **Plot J-V Curve Button:** Opens a separate window to display and export calculated light and dark J-V curves.

## 3.6 Buttons and Menu Actions (Summary)

Key action buttons are distributed across the panels:

- **Add Layer:** Adds a new layer to the stack.
- **Run Optical Calculation:** Performs TMM simulation.
- **Calculate Device Parameters:** Performs detailed balance simulation.
- **Plot J-V Curve:** Opens the J-V plotting window.
- **Export Optical Profile:** Saves R, T, A data to CSV.
- **Export Generation Function:** Saves calculated generation profile(s) to CSV.
- **Save/Load Simulation:** Saves/loads the complete simulation state (`.soley` file).
- **Optimize Optical Stack:** Opens the layer thickness optimisation window.
- **Define Batch Calculations:** Opens the batch parameter sweep definition window.
- **Absorber 1..6 (SRH):** Opens the defect definition window for the specific absorber.
- **Update Bandgap:** Applies manually entered bandgap values.

There are no traditional File/Edit menus; all actions are controlled via buttons in the main interface.

# 4 Methodology and Theoretical Background

This section describes the physical models and assumptions used within SOLEY.

## 4.1 Optical Model: Transfer Matrix Method (TMM)

SOLEY calculates how light interacts with the solar cell stack using the Transfer Matrix Method (TMM).

### 4.1.1 Core Equations

The TMM models each layer with a characteristic matrix. Light propagation across an interface between layer $j$ and $j+1$ is described by an interface matrix $D_j$. Propagation through a layer $j$ of thickness $d_j$ is described by a propagation matrix $P_j$.

For a stack of $N$ layers, the total transfer matrix $M$ is the product of these individual matrices:

$$M = D_0 \cdot P_1 \cdot D_1 \cdot P_2 \cdot \cdots \cdot P_N \cdot D_N \tag{6}$$

where $D_0$ represents the interface from the incident medium (e.g., air) to the first layer, and $D_N$ represents the interface from the last layer to the substrate or exit medium.

From the elements of the total matrix $M = \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix}$, the complex reflection coefficient $r$ and transmission coefficient $t$ are found:

$$r = \frac{M_{21}}{M_{11}} \tag{7}$$

$$t = \frac{1}{M_{11}} \tag{8}$$

Reflectance (R) and Transmittance (T) are then calculated as:

$$R = |r|^2 \tag{9}$$

$$T = \mathrm{Re}\left(\frac{k_{z,N+1}}{k_{z,0}}\right)|t|^2 \quad \text{(TE)} \quad \text{or} \quad T = \mathrm{Re}\left(\frac{k_{z,N+1}n_0^2}{k_{z,0}n_{N+1}^2}\right)|t|^2 \quad \text{(TM)} \tag{10}$$

where $k_z$ is the wavevector component perpendicular to the interfaces, and $n$ is the refractive index of the incident (0) and exit (N+1) media. Absorbance (A) in the stack is calculated as $A = 1 - R - T$. Absorbance within a specific layer is found by calculating the Poynting vector difference at its boundaries.

### 4.1.2 Handling of Coherent/Incoherent Layers

SOLEY implicitly assumes coherent light propagation throughout the stack, which is standard in TMM. For very thick layers where incoherence might occur (e.g., thick substrates), the TMM approach still provides a good approximation for overall R, T, and A, although it does not explicitly model phase scrambling. SOLEY includes numerical stability enhancements for thick layers.

### 4.1.3 Assumptions

- Layers are optically homogeneous and isotropic.
- Interfaces between layers are perfectly planar and parallel.
- Light propagation is coherent within the entire stack.
- Material optical constants (n, k) are known for the simulated wavelength range.

## 4.2 Layer Mixing: Bruggeman Effective Medium Approximation

When the 'Mix' option is enabled for a layer, SOLEY uses the Bruggeman Effective Medium Approximation (EMA) to calculate the effective optical constants of the mixture between that layer and the one below it.

### 4.2.1 Governing Equation

The Bruggeman EMA solves the following equation for the effective dielectric permittivity $\epsilon_{eff}$ of a two-component mixture:

$$f_1\frac{\epsilon_1 - \epsilon_{eff}}{\epsilon_1 + 2\epsilon_{eff}} + f_2\frac{\epsilon_2 - \epsilon_{eff}}{\epsilon_2 + 2\epsilon_{eff}} = 0 \tag{11}$$

where $f_1, f_2$ are the volume fractions of material 1 and 2 ($f_1 + f_2 = 1$), and $\epsilon_1, \epsilon_2$ are their respective complex dielectric permittivities ($\epsilon = (n + ik)^2$). SOLEY solves this equation iteratively at each wavelength to find $\epsilon_{eff}$, from which the effective $n_{eff}$ and $k_{eff}$ are derived.

### 4.2.2 Assumptions

- The mixture is random and homogeneous on a macroscopic scale.
- The inclusions (minority component) are roughly spherical.
- The size of the inclusions is much smaller than the wavelength of light.

## 4.3 Electrical Model: Detailed Balance + Recombination

SOLEY uses a detailed balance approach, similar to the Shockley-Queisser limit, but extended to include non-radiative recombination and resistive losses.

### 4.3.1 Core Equation (Diode Equation Basis)

The current-voltage (J-V) characteristic of each subcell (absorber) is modelled using a diode equation:

$$J(V) = J_{ph} - J_{rec}(V) - J_{shunt}(V) \tag{12}$$

where $J_{ph}$ is the photogenerated current density (calculated from optical absorption), $J_{rec}(V)$ is the voltage-dependent recombination current density, and $J_{shunt}(V)$ represents current loss through shunt pathways. The terminal voltage is related to the internal junction voltage $V_j$ by series resistance $R_s$: $V = V_j - J \cdot R_s$.

The recombination current is the sum of different mechanisms:

$$J_{rec}(V_j) = J_{0,rad}\left(e^{\frac{qV_j}{kT}} - 1\right) + J_{0,Auger}\left(e^{\frac{qV_j}{kT}} - 1\right) + J_{0,SRH}(V_j)\left(e^{\frac{qV_j}{n_{SRH}kT}} - 1\right) \tag{13}$$

where $J_0$ terms are saturation current densities for radiative, Auger, and SRH recombination, $k$ is Boltzmann's constant, $T$ is temperature, $q$ is elementary charge, and $n_{SRH}$ is the SRH ideality factor. Note that $J_{0,SRH}$ can be voltage-dependent if a custom equation is used, but the recombination paths by default do not depend on the voltage.

The shunt current is modelled as $J_{shunt}(V) = (V + J \cdot R_s)/R_{sh}$, where $R_{sh}$ is the shunt resistance.

SOLEY solves the implicit equation for J at each V numerically to obtain the J-V curve.

### 4.3.2 Calculation of Jsc

The short-circuit current density $J_{sc}$ is ideally equal to $J_{ph}$. $J_{ph}$ is calculated by integrating the absorbed photon flux above the bandgap $E_g$ for each absorber layer, using the generation profile from the TMM simulation:

$$J_{ph} = q \int_{E_g}^{\infty} \Phi_{abs}(E) dE \tag{14}$$

where $\Phi_{abs}(E)$ is the absorbed photon flux per unit energy. SOLEY calculates this from the layer absorbance $A(\lambda)$ and the incident spectrum $\Phi_{in}(\lambda)$:

$$J_{ph} = q \int_{\lambda_{min}}^{\lambda_{max}} A(\lambda)\Phi_{in}(\lambda)d\lambda \tag{15}$$

where the integral is performed over wavelengths corresponding to energies above $E_g$. The effective $J_{sc}$ used in calculations accounts for early recombination onset and resistive losses near V=0.

### 4.3.3 Calculation of Voc

The open-circuit voltage $V_{oc}$ is the voltage where the net current $J(V)$ is zero. It is found by solving:

$$J_{ph} = J_{rec}(V_{oc}) + J_{shunt}(V_{oc}) \tag{16}$$

This equation is solved numerically by SOLEY.

### 4.3.4 Recombination Mechanisms

- **Radiative (J0_rad):** Calculated based on detailed balance, assuming the cell emits blackbody radiation filtered by its absorptivity above the bandgap. The equation used is:

$$J_{0,rad} = \frac{1}{f}\frac{2\pi q(kT)^3}{h^3c^2}\int_{x_g}^{\infty}\frac{x^2}{e^x-1}dx \approx \frac{1}{f}\frac{2\pi q(kT)^3}{h^3c^2}e^{-x_g} \tag{17}$$

  where $x_g = E_g/kT$, $h$ is Planck's constant, $c$ is the speed of light, and $f$ is the étendue factor (geometry factor, $1.09 \times 10^{-5}$ for 1 sun from the SQ paper).

- **Auger (J0_auger):** Represents three-particle recombination. The saturation current $J_{0,Auger}$ depends on the Auger coefficients $(C_n, C_p)$, intrinsic carrier concentration $(n_i)$, doping concentration $(N_{dop})$, and layer thickness $(d)$:

$$J_{0,Auger} \approx q \cdot d \cdot C_{maj} \cdot N_{dop}^2 \cdot n_i \tag{18}$$

  where $C_{maj}$ is the coefficient for the majority carrier ($C_p$ for p-type, $C_n$ for n-type). SOLEY uses user-provided $C_n$ and $C_p$ values and includes temperature and bandgap dependencies for these coefficients.

- **Shockley-Read-Hall (SRH):** Recombination via defect states within the bandgap. SOLEY offers two ways to define $J_{0,SRH}$ and its ideality factor $n_{SRH}$:

  1. **Microscopic Parameters (Scaffidi Model):** Calculates $J_{0,SRH}$ from fundamental defect parameters (trap density $N_t$, capture cross-section $\sigma$, thermal velocity $v_{th}$, trap energy level $E_t$, doping, built-in voltage $V_{bi}$, etc.) and interface recombination velocity $(S_p)$. It calculates bulk $(J_{00,bulk})$ and interface $(J_{00,interface})$ prefactors and uses an activation energy $(E_a)$ approach:

$$J_{00,bulk} \propto N_t \cdot \sigma \cdot v_{th} \cdot \sqrt{N_c N_v / N_{dop}} \tag{19}$$

$$J_{00,interface} \propto S_p \cdot N_{dop} \tag{20}$$

$$J_{0,SRH} = (J_{00,bulk} + J_{00,interface}) \exp\left(-\frac{E_a}{n_{SRH}kT}\right) \tag{21}$$

*Assumptions:* Single dominant trap level, specific model for depletion width and interface recombination. This is mostly based on Cuevas' work.

2. **Custom Equation:** Allows the user to define $J_{0,SRH}$ as an arbitrary function of voltage ($V$) and other material/device parameters using Python syntax. This provides maximum flexibility to implement custom or empirical recombination models.

### 4.3.5 Inclusion of Series and Shunt Resistance

Series resistance ($R_s$) reduces the output voltage and fill factor. Shunt resistance ($R_{sh}$) provides an alternative path for current, reducing $V_{oc}$ and fill factor. SOLEY includes these as lumped parameters in the diode equation, affecting the terminal voltage and current.

### 4.3.6 Multijunction Simulation (2-Terminal)

For devices with multiple absorbers, SOLEY assumes a 2-terminal configuration. It calculates the J-V curve for each subcell individually. The overall device J-V curve is then determined by the principle of current matching: the total current density cannot exceed the lowest $J_{sc}$ among the series-connected subcells. The total $V_{oc}$ is the sum of the individual subcell $V_{oc}$ values (assuming negligible recombination at tunnel junctions). The fill factor and efficiency are calculated for the current-limited multijunction device.

## 4.4 Limitations and Hypotheses

Users should be aware of the inherent assumptions and limitations:

- **1D Simulation:** SOLEY assumes infinite lateral extent and uniformity. It cannot model edge effects, localised defects, or non-uniform illumination.
- **Simplified Transport:** The detailed balance model does not explicitly calculate carrier concentration profiles or electric fields within the device like drift-diffusion solvers do. Transport is implicitly handled via recombination parameters and ideal collection assumptions (modified by resistance).
- **SRH Model Assumptions:** When using the Scaffidi model, it assumes a single, dominant trap level and specific forms for bulk and interface recombination. The custom $J_0$ approach relies entirely on the user's input model.
- **Interface Modelling:** Interfaces are treated primarily through their optical properties (TMM) and potentially via interface recombination terms ($J_{00,interface}$ or custom $J_0$). Detailed interface physics (band alignment, interface dipoles, specific interface traps) are not explicitly modelled as in drift-diffusion.
- **Thermal Effects:** Temperature is a fixed input parameter. SOLEY does not calculate self-heating effects within the device during operation.
- **Coherence Assumption:** TMM assumes coherent light propagation, which may not be fully accurate for very thick, non-specular layers. That's why I added the smoothing functionality, and some numerical stability enhancements. It works decently for thick Silicon layers and silicon solar cells can normally be modelled properly.

# 5 Optical Simulation Module Details

This section provides more detail on the optical calculations performed by SOLEY.

## 5.1 TMM Implementation Specifics

SOLEY uses a standard recursive TMM algorithm. To handle potentially thick or highly absorbing layers where numerical overflow or underflow can occur in the propagation matrix calculation ($e^{\pm ik_z d}$), the implementation includes:

- **Scaling:** If the imaginary part of the exponent $k_z d$ becomes too large (e.g., ¿ 350), the exponent is scaled down before calculating the exponential, and a corresponding scaling factor is applied to the matrix elements to maintain correctness while avoiding extreme values.
- **Sublayering (Experimental):** For very thick absorbing layers, the propagation matrix calculation can optionally be split into multiple sub-steps to improve stability, although this increases computation time. This is handled internally based on layer thickness and absorption coefficient.
- **Parallel Processing:** Optical calculations (R, T, A) for each wavelength are independent. SOLEY utilises multiprocessing to distribute these calculations across available CPU cores, significantly speeding up the simulation, especially for wide wavelength ranges or fine steps.

## 5.2 Defining Optical Constants (n, k file format)

Each layer requires a file containing its optical constants (refractive index $n$ and extinction coefficient $k$).

- **Format:** The file must be a plain text file (`.txt`).
- **Columns:** It should contain three columns of numerical data separated by whitespace (spaces or tabs):
  1. Wavelength (in nanometres, nm)
  2. Refractive Index ($n$, unitless)
  3. Extinction Coefficient ($k$, unitless)
- **Order:** Wavelengths should preferably be sorted in ascending order.
- **Comments:** Lines starting with '%' are ignored as comments.
- **Location:** It is recommended to keep these files in a subfolder named `Optical_Indices` within the SOLEY application directory or the directory where simulation files are saved/loaded. SOLEY will search in multiple locations (relative to the simulation file, relative to the executable, standard folders) to find the required files.

SOLEY uses linear interpolation to find $n$ and $k$ values at wavelengths required for the simulation that may fall between the points defined in the file. Extrapolation is used for wavelengths outside the defined range.

## 5.3 Calculating Reflectance, Transmittance, and Absorbance

After running the optical calculation:

- **Reflectance (R):** The fraction of incident light intensity reflected from the front surface of the device stack.
- **Transmittance (T):** The fraction of incident light intensity transmitted through the entire device stack.
- **Absorbance (A):** Calculated in two ways:
  - **Total Stack Absorbance:** Calculated as $1 - R - T$.
  - **Layer-Specific Absorbance:** Calculated for layers where the 'Calc A' checkbox is ticked. This is done by computing the difference in the Poynting vector (energy flow) at the front and back interfaces of that specific layer, normalised by the incident Poynting vector. This represents the fraction of incident light absorbed only within that layer.

The results are plotted against wavelength in the main plotting area.

## 5.4 Calculating Generation Profiles

The optical generation rate $G(x, \lambda)$ (photons generated per unit volume per unit time per unit wavelength) at a position $x$ within a layer is proportional to the local light intensity $I(x, \lambda)$ and the absorption coefficient $\alpha(\lambda)$ of the material at that wavelength:

$$G(x, \lambda) \propto \alpha(\lambda) \cdot I(x, \lambda) \tag{22}$$

SOLEY calculates the electric field profile $E(x, \lambda)$ within each layer using the TMM results. The local intensity is $I(x, \lambda) \propto |E(x, \lambda)|^2$. The absorption coefficient is $\alpha(\lambda) = 4\pi k(\lambda)/\lambda$.

The total generation rate $G_{tot}(x)$ (photons/m$^3$/s) at position $x$ is obtained by integrating over the incident spectrum $\Phi_{in}(\lambda)$ (photons/m$^2$/s/nm):

$$G_{tot}(x) = \int_{\lambda_{min}}^{\lambda_{max}} \frac{\alpha(\lambda) I(x, \lambda)}{I_{in}(\lambda)} \Phi_{in}(\lambda) d\lambda \tag{23}$$

where $I_{in}(\lambda)$ is the incident intensity used for normalisation within the TMM calculation. SOLEY performs this calculation numerically for layers marked with 'Calc A'.

### 5.4.1 Direct Illumination

Calculates the generation profile assuming a single angle of incidence specified by the user.

### 5.4.2 Diffuse Illumination

Calculates the generation profile assuming light arrives equally from all directions in a hemisphere. This involves:

- Calculating the intensity profile $I(x, \lambda, \theta)$ for multiple incidence angles $\theta$.

- Performing a weighted average over these angles, typically weighted by $\sin(2\theta)$ to account for the solid angle and Lambertian distribution.
- Integrating the angle-averaged generation rate over the incident spectrum.

The number of angle steps used for the approximation is set in the GUI.

## 5.5 Handling Polarisation and Angle of Incidence

- **Polarisation:** TMM calculations are performed separately for TE (s-polarisation) and TM (p-polarisation) components of light, as the interface Fresnel coefficients differ. For 'Unpolarised' light, SOLEY calculates both TE and TM results and averages them: $Result_{unpol} = (Result_{TE} + Result_{TM})/2$. At normal incidence (0 degrees), TE and TM results are identical, so only one calculation is needed.
- **Angle of Incidence:** The angle $\theta$ (relative to the surface normal) affects the wavevector components $(k_x, k_z)$ within each layer via Snell's Law, which modifies the TMM matrices. SOLEY correctly accounts for this angle dependence.

## 5.6 Data Smoothing (Savitzky-Golay Filter)

Optical interference effects can cause rapid oscillations in the calculated R, T, and A spectra when a layer is very thick. This particularly problematic when using a glass substrate or superstrate, for example.

- If 'Enable Smoothing' is checked, SOLEY applies a Savitzky-Golay filter to the calculated R, T, and A data after the TMM calculation.
- This filter fits a polynomial to a window of data points, effectively smoothing out high-frequency noise or interference fringes while preserving broader spectral features.
- The 'Window Length' (must be odd) and 'Polynomial Order' parameters control the degree of smoothing. Larger windows or lower orders result in more smoothing.
- Smoothing is applied only for display and export; the underlying electrical calculations typically use the unsmoothed absorbance data for accuracy.
- Smoothing is honestly just a plan B when you have very thick layer, to avoid those crazy interferences. It's not the best, but it kind of works. I guess. Not great not terrible.

## 5.7 Exporting Optical Profile and Generation Data

- **Export Optical Profile:** Saves the currently plotted R, T, and layer-specific A values (after any smoothing) versus wavelength to a CSV file.
- **Export Generation Function:** Calculates the depth-dependent total generation rate $G_{tot}(x)$ (photons/$m^3$/s) within the layers marked 'Calc A', integrated over the selected incident spectrum. The calculation uses either direct or diffuse illumination based on the GUI setting. The results (Position (nm), Generation Rate) are saved to a CSV file, with positions spanning continuously across all layers in the stack. This calculation uses multiprocessing for efficiency.

# 6 Electrical Device Modelling Module Details

This section explains the electrical simulation components in more detail.

## 6.1 Detailed Balance Model Implementation Specifics

SOLEY calculates the current density $J$ at a given voltage $V$ by balancing the photogenerated current ($J_{ph}$) against recombination currents ($J_{rec}$) and shunt losses ($J_{shunt}$). It solves the implicit diode equation numerically:

$$J = J_{ph} - J_{rec}(V_j) - \frac{V_j}{R_{sh}} \quad \text{where } V_j = V + J \cdot R_s \tag{24}$$

The numerical solver finds the value of $J$ that satisfies this equation for each $V$. $J_{ph}$ is determined directly from the optical simulation results (Section 5.4).

## 6.2 Calculation of Jsc, Voc, FF, and Efficiency

These key parameters are derived from the calculated J-V curve:

- **Jsc (Short-Circuit Current Density):** Calculated as the current density $J$ when the voltage $V = 0$. It is primarily determined by $J_{ph}$ but slightly reduced by recombination and shunt losses even at zero bias.
- **Voc (Open-Circuit Voltage):** The voltage $V$ where the net current density $J = 0$. Found by solving $J_{ph} = J_{rec}(V_{oc}) + J_{shunt}(V_{oc})$ numerically.
- **FF (Fill Factor):** A measure of the squareness of the J-V curve. Calculated by finding the maximum power point ($P_{max} = V_{mp} \times J_{mp}$) on the J-V curve:

$$FF = \frac{V_{mp} \times J_{mp}}{V_{oc} \times J_{sc}} \tag{25}$$

- **Efficiency ($\eta$):** The ratio of the maximum output power to the total incident power ($P_{in}$) from the selected spectrum:

$$\eta = \frac{P_{max}}{P_{in}} = \frac{V_{oc} \times J_{sc} \times FF}{P_{in}} \tag{26}$$

  $P_{in}$ is calculated by integrating the power density of the input spectrum file over photon energy.

## 6.3 Recombination Mechanisms In-Depth

SOLEY models three main recombination pathways contributing to $J_{rec}$.

### 6.3.1 Radiative Recombination Parameters

- **f factor (Étendue):** This input parameter scales the radiative recombination current $J_{0,rad}$. It is only accessible through batch calculations (I removed the input box in the main GUI quite late, I could put it back if there is demand). The default value ($1.09 \times 10^{-5}$) corresponds to the standard Shockley-Queisser limit for 1 sun illumination.

- **Temperature (T):** Affects $J_{0,rad}$ strongly through the $T^3$ term and the exponential dependence on $E_g/kT$.
- **Bandgap (Eg):** Directly determines the energy threshold for radiative emission, impacting $J_{0,rad}$ exponentially.

### 6.3.2 Auger Recombination Parameters

- **Electron/Hole Auger Coefficients (Cn, Cp):** These inputs (in $cm^6/s$) define the strength of the Auger process for each absorber. They are used to calculate $J_{0,Auger}$.
- **Temperature and Bandgap Dependence:** SOLEY includes empirical scaling factors for $C_n$ and $C_p$ based on temperature and bandgap, refining the $J_{0,Auger}$ calculation.
- **Doping Concentration (Ndop):** $J_{0,Auger}$ calculation uses the doping concentration defined in the SRH Defect Parameter window (`Ndop_abs`) to account for majority carrier density.

### 6.3.3 SRH Recombination (Defect Parameter Window Details)

This window allows detailed control over Shockley-Read-Hall recombination for each absorber.

- **Using the Scaffidi Model:**
  - Input microscopic parameters: $N_t$ (trap density), $\sigma_n$ (capture cross-section), $v_{th}$ (thermal velocity), $N_c$, $N_v$, $N_{dop}$, $V_{bi}$, $\epsilon$ (permittivity) for the absorber, and $S_p$ (interface recombination velocity), $N_{c,adj}$, $N_{dop,adj}$, $\theta$ for the adjacent layer interface.
  - Click **Compute J00 Bulk** and **Compute J00 Interface** to calculate the respective prefactors based on the model equations (shown in the window).
  - Input the **Activation Energy (Ea)** and **Ideality Factor (n)** for the SRH process.
  - Click **Compute J0_SRH**. SOLEY calculates the final $J_{0,SRH}$ at V=0 using the $J_{00}$ values, Ea, n, and T. The resulting $J_{0,SRH}$ ($mA/cm^2$) and $n$ factor are displayed and stored.
  - The calculated carrier lifetime ($\tau = 1/(v_{th}\sigma_n N_t)$) is also displayed.
- **Defining Custom J0 Equations:**
  - Enter a mathematical expression for $J_{0,SRH}$ (in $A/m^2$) in the **Custom J0 Definition** text box.
  - The expression can use standard Python math functions (e.g., `np.exp`, `np.sqrt`) and available variables (listed in the window, e.g., `V`, `T`, `E_g`, `Rs`, `n`, `Ndop_abs`, etc.). Note that variables are automatically converted to SI units for the calculation.
  - Click **Define Custom Recombination**.

  - If the equation contains 'V', it defines a voltage-dependent $J_{0,SRH}(V)$. A plot of $J_{0,SRH}(V)$ vs V will be shown.
  - If 'V' is not present, the equation defines a constant $J_{0,SRH}$ value, which is displayed.
  - This custom $J_{0,SRH}$ (or $J_{0,SRH}(V)$) is then used in the main device calculation instead of the Scaffedi model result.

- **Saving:** Click **Save & Close** to store the calculated or defined $J_{0,SRH}$ and $n$ factor (along with all input parameters) for the selected absorber. These values will then be used in the main device simulation.

## 6.4 Calculation of J-V Curves (Light and Dark)

- Clicking the **Plot J-V Curve** button opens a dedicated window.
- SOLEY calculates the current density $J$ for a range of voltage points $V$ (defined by the user in the J-V window) by numerically solving the diode equation described in Section 6.1.
- **Light J-V:** Includes the photogenerated current $J_{ph}$.
- **Dark J-V:** Calculates the curve with $J_{ph} = 0$. This can be optionally displayed alongside the light curve.
- The window allows adjusting the plot axes (V min/max, J min/max) and exporting the plotted data to a CSV file.

## 6.5 Multijunction Device Simulation Logic

- SOLEY calculates the individual J-V characteristics and performance parameters ($V_{oc,i}, J_{sc,i}, FF_i, \eta_i$) for each absorber layer $i$ defined in the stack.
- For the 2-terminal multijunction device, it assumes the subcells are connected in series.
- The overall short-circuit current $J_{sc,MJ}$ is limited by the subcell with the *lowest* $J_{sc,i}$: $J_{sc,MJ} = \min(J_{sc,i})$.
- The overall open-circuit voltage $V_{oc,MJ}$ is the sum of the individual subcell voltages: $V_{oc,MJ} = \sum V_{oc,i}$.
- The multijunction Fill Factor ($FF_{MJ}$) and Efficiency ($\eta_{MJ}$) are calculated based on these combined $J_{sc,MJ}$ and $V_{oc,MJ}$ values, using an approximation for the combined J-V curve shape.
- The results for the multijunction device are displayed in the final row of the device results table.

# 7 Multijunction Solar Cell J-V Calculation Methodology

## 7.1 Physical Principles

In a series-connected multijunction solar cell, the subcells are constrained to operate at the same current density, while their voltages add up to give the total device voltage. This arrangement can be represented as:

$$J_{\mathrm{MJ}}(V) = J_1(V_1) = J_2(V_2) = \ldots = J_n(V_n) \tag{27}$$

$$V_{\mathrm{MJ}} = \sum_{i=1}^{n} V_i \tag{28}$$

where $J_{\mathrm{MJ}}$ is the multijunction current density, $V_{\mathrm{MJ}}$ is the multijunction voltage, and $J_i(V_i)$ is the current density at voltage $V_i$ for subcell $i$.

## 7.2 Computational Approach

To calculate the multijunction J-V curve, we invert the typical approach. Rather than computing $J(V)$, we compute $V(J)$ for each subcell and sum them:

1. Define a common current axis $J_{\mathrm{common}}$ from a negative value (typically $-0.5 \times J_{\mathrm{sc,min}}$) to slightly above the minimum $J_{\mathrm{sc}}$ value among subcells.
2. For each current point $J_j$ on this axis:
   (a) For each subcell $i$, calculate the voltage $V_{i,j}$ that produces current $J_j$
   (b) The total voltage at this current is $V_{\mathrm{MJ},j} = \sum_{i=1}^{n} V_{i,j}$
3. This yields the multijunction J-V relationship as a set of points $(V_{\mathrm{MJ},j}, J_j)$

## 7.3 Mathematical Formulation

For each subcell, the current-voltage relationship follows the diode equation extended with additional recombination terms and parasitic resistances:

$$J(V) = J_{\mathrm{sc}} - J_0 \left( \exp\left( \frac{q(V + JR_s)}{nkT} \right) - 1 \right) - \frac{V + JR_s}{R_{\mathrm{sh}}} \tag{29}$$

where $J_{\mathrm{sc}}$ is the short-circuit current density, $J_0$ is the reverse saturation current density (combining radiative, Auger, and SRH recombination), $n$ is the ideality factor, $R_s$ is the series resistance, and $R_{\mathrm{sh}}$ is the shunt resistance.

To solve for $V(J)$, we rearrange this equation and define an implicit function:

$$f(V, J) = J - J_{\mathrm{sc}} + J_0 \left( \exp\left( \frac{q(V + JR_s)}{nkT} \right) - 1 \right) + \frac{V + JR_s}{R_{\mathrm{sh}}} = 0 \tag{30}$$

For each current value $J$, we numerically solve $f(V, J) = 0$ for $V$ using a combination of:

- Bracketing methods (e.g., `brentq`)
- Newton's method with intelligent initial guesses
- Adaptive boundary selection based on shunt resistance values

## 7.4 Fill Factor Calculation

With an accurately calculated J-V curve, the fill factor can be determined directly from the maximum power point:

$$FF_{\text{MJ}} = \frac{P_{\max}}{J_{\text{sc,MJ}} \times V_{\text{oc,MJ}}} = \frac{J_{\text{mp}} \times V_{\text{mp}}}{J_{\text{sc,MJ}} \times V_{\text{oc,MJ}}} \tag{31}$$

where $J_{\text{mp}}$ and $V_{\text{mp}}$ are the current density and voltage at the maximum power point.

## 7.5 Advantages

This methodology offers several significant advantages:

- **Physically accurate:** By directly modelling the series constraint, it captures the exact behaviour of series-connected multijunction cells.
- **Handles non-ideal effects:** Incorporates series and shunt resistances, as well as different recombination mechanisms, allowing for realistic device modelling.
- **Numerical robustness:** The adaptive approach to solving the implicit equation handles challenging cases like very low shunt resistances.
- **Direct parameter extraction:** Accurately determines key performance parameters ($J_{\text{sc}}$, $V_{\text{oc}}$, FF, efficiency) from the full J-V curve.

## 7.6 Limitations

The method also has some limitations:

- **Computational intensity:** Requires solving many implicit equations numerically, which can be more computationally expensive. I tried with semi-empirical formula such as extending Green's formula, but never got a satisfactory result. And honestly it is already quite fast.
- **Convergence challenges:** For extreme parameter values (very low shunt resistance or very high series resistance), numerical methods may not converge.
- **Temperature gradients:** Does not account for potential temperature differences between subcells under illumination.
- **Interface recombination:** Tunnel junction properties between subcells are not explicitly modeled. Yet. Let's see.

## 7.7 Extensions and Refinements

The model can be extended to include:

- Explicit tunnel junction resistance between subcells
- Non-linear shunt conduction
- Photon recycling
- Carrier injection-dependent series resistance effects maybe? Not a priority though.

# 8 Advanced Features

SOLEY includes features for optimisation and systematic parameter exploration.

## 8.1 Layer Thickness Optimisation

This feature helps find the layer thicknesses that maximise the 2-terminal multijunction efficiency. Or for optimising an Anti-reflective coating for example.

- Access via the **Optimize Optical Stack** button.
- A window appears listing all layers in the stack.
- **Setting Parameters:** For each layer you want to optimise:
  - Check the **Optimize** box.
  - Enter the **Min Thickness** and **Max Thickness** (nm) range to explore.
  - Enter the number of **Steps** (at least 2) to divide the thickness range into. More steps give higher resolution but take longer.
- **Algorithm:** SOLEY performs a grid search. It calculates the device efficiency for every possible combination of thicknesses defined by the selected layers and their steps.
- **Second Stage Refinement (Optional):** If checked, SOLEY performs a second, finer grid search around the best point found in the first stage. This can improve accuracy but increases calculation time.
- **Running:** Click **Run Optimization**. A progress window shows the status. This can be time-consuming for many layers or steps.
- **Interpreting Results:** A results window displays the best multijunction efficiency found and the corresponding optimal thicknesses for the selected layers. It also shows the original thicknesses for comparison. Results can be copied to the clipboard.

## 8.2 Batch Calculations

This feature allows automated simulation runs while systematically varying one or more parameters. It doesn't yet implement a logarithmic progression like SCAPS does, but this will be included very soon!

- Access via the **Define Batch Calculations** button.
- **Main Batch Window:**
  - Select **General Parameters** (Temperature, f factor) to vary by checking their box. Enter Start, End, and Steps values for the parameter sweep.
  - Click on an **Absorber** button (**Absorber 1** to **Absorber 6**) to define parameter sweeps specific to that absorber.
- **Absorber Batch Window:**
  - Select parameters specific to this absorber (e.g., Rs, Rsh, Auger coefficients, SRH microscopic parameters like Ea, Nt, Sp) by checking their box.
  - Enter Start, End, and Steps values for each selected parameter.
  - Click **Save Batch** to confirm settings for this absorber. A green indicator appears next to the absorber button in the main batch window if any parameters are set for batch variation.
- **Running Batch Jobs:**
  - In the main batch window, click **Run Batch Calculation**.
  - SOLEY calculates the device performance for every combination of the selected varying parameters.
  - A progress window shows the status and logs results for each combination.
- **Saving and Interpreting Results:**
  - After completion, SOLEY prompts you to save two CSV files:
    1. **PV Parameters Data:** Contains one row per parameter combination. Columns include the values of the varied parameters and the resulting device metrics (Voc, Jsc, FF, Eff) for each subcell and the multijunction device.
    2. **JV Curves Data:** Contains the calculated J-V curves for each subcell and the multijunction device for every parameter combination.
  - These files can be imported into data analysis software (e.g., Excel, Python Pandas) to analyse trends and identify optimal parameter sets.

## 8.3 Saving and Loading Simulation States

- **Save Simulation:** Click this button to save the entire state of the simulation, including:
  - The layer stack definition (filenames, thicknesses, flags).

- All calculation parameters (wavelength, angle, etc.).
- All device modelling parameters (spectrum file, T, f, resistances, Auger coeffs, bandgaps, SRH defect parameters).

The data is saved in a single `.soley` file (JSON format).

- **Load Simulation:** Click this button to load a previously saved `.soley` file. SOLEY will attempt to restore the complete simulation state. It will search for the required optical constant and spectrum files based on stored paths and standard locations. If a file cannot be found, it will prompt the user to locate it manually. After loading, the optical calculation is automatically re-run.

## 8.4 Simulating Diffuse Light Effects

- Check the **Diffuse Light** box in the Calculation Parameters panel.
- Specify the number of **Angle Steps** to use for approximating hemispherical incidence (e.g., 5-18 steps). More steps increase accuracy but also calculation time.
- When **Run Optical Calculation** is clicked, SOLEY calculates R, T, and A by averaging the results over the specified angles, weighted appropriately for diffuse light ($\propto \sin(2\theta)$).
- The **Export Generation Function** button will also calculate the generation profile considering the diffuse illumination.
- Device electrical parameters are then calculated using the absorbance results obtained under diffuse illumination.

# 9 File Formats

SOLEY uses specific file formats for input and output data.

## 9.1 Optical Constant Files (`.txt`)

These files provide the refractive index ($n$) and extinction coefficient ($k$) for each layer material.

- **Format:** Plain text (`.txt`).
- **Content:** Three columns separated by whitespace (space or tab).
  1. Wavelength (nm)
  2. Refractive Index $n$ (unitless)
  3. Extinction Coefficient $k$ (unitless)
- **Comments:** Lines starting with '%' are ignored.
- **Example:**

```
% Example Optical Constant File for Material X
Wavelength(nm) n       k
300            1.5     0.01
310            1.51    0.012
...            ...     ...
1200           1.45    0.001
```

## 9.2 Spectrum Files (`.txt`)

These files define the incident light spectrum used in electrical calculations.

- **Format:** Plain text (`.txt`).
- **Content:** Two columns separated by whitespace.
  1. Wavelength (nm)
  2. Spectral Irradiance ($W/m^2/nm$)
- **Comments:** Lines starting with '%' are ignored.
- **Example:**

```
% Example AM1.5G Spectrum
Wavelength(nm) Irradiance(W/m2/nm)
300            0.05
305            0.15
...            ...
1200           0.8
```

## 9.3 Simulation State Files (`.soley` JSON structure)

These files save the complete state of a simulation.

- **Format:** JSON (`.json` or `.soley`).
- **Content:** A structured text file containing all GUI settings:
  - Layer definitions (optical file paths, thicknesses, flags).
  - Calculation parameters (wavelength range, angle, polarisation, smoothing).
  - Device parameters (spectrum file path, T, f, injection factor, resistances, Auger coeffs, bandgaps).
  - SRH defect parameters (microscopic values, custom equations if used).
- **Purpose:** Allows users to save their work and reload it later, ensuring reproducibility. SOLEY attempts to find linked optical/spectrum files based on saved paths and relative locations.

## 9.4 Exported CSV File Formats

SOLEY can export various results into Comma Separated Value (`.csv`) files.

- **Optical Profile:** Columns for Wavelength (nm), R, T, and A_*LayerName* for each layer where absorbance was calculated.
- **Generation Function:** Columns for Layer Name, Position (nm) across the stack, and Generation Rate (Photon/$m^3$/s).
- **J-V Curves:** Columns for Voltage (V) and Current Density (mA/$cm^2$) for each absorber's light and dark curves (if plotted). Data is interpolated onto a common voltage axis.
- **Batch Results (PV Parameters):** Columns for each varied parameter, followed by columns for Eg, Voc, Jsc, FF, Eff for each subcell and the multijunction device for every parameter combination.
- **Batch Results (JV Curves):** Columns for Voltage (V), followed by pairs of Current Density (mA/$cm^2$) columns for each subcell/multijunction device for every parameter combination.

# 10 Troubleshooting and FAQ

This section addresses common issues and questions.

## 10.1 Common Errors and Solutions

- **Error: "Cannot find optical data file: [filename]"**
  - **Cause:** SOLEY cannot locate the required `.txt` file for a layer's optical constants.
  - **Solution:** Ensure the file exists and is accessible. Place optical files in an `Optical_Indices` subfolder near the SOLEY executable or the saved `.soley` file. If loading a simulation, SOLEY will prompt you to locate missing files manually. Verify the filename in the layer list is correct.
- **Error: "No incident spectrum file."**
  - **Cause:** Attempting to run device calculations or export generation profiles without selecting a spectrum file in the Device Modelling Panel.
  - **Solution:** Click 'Browse' next to 'Spectrum File' and select a valid spectrum `.txt` file.
- **Error: "No layers defined for simulation" / "No absorber layers selected."**
  - **Cause:** Trying to run calculations without adding layers or without marking at least one layer as an 'Absorber'.
  - **Solution:** Add layers using the 'Add Layer' button. Check the 'Absorber' box for the relevant layer(s) in the Layer List Panel.

- **Error during calculations (e.g., ValueError, LinAlgError, Brentq failure)**
  - **Cause:** Often due to invalid input parameters (e.g., non-numeric values, zero thickness, extreme resistance values) or numerical instability in the TMM or device solvers. Can also occur with highly unusual optical constants or extremely thin/thick layers.
  - **Solution:** Double-check all input parameters in the GUI, especially thicknesses, resistances, Auger coefficients, and SRH parameters. Ensure optical constant files are valid. Try slightly adjusting layer thicknesses or the wavelength step. If using custom SRH equations, verify their numerical stability. Check console output for more specific error messages if running from source.
- **GUI unresponsive during long calculations (Optimisation, Batch)**
  - **Cause:** Intensive calculations run in separate threads, but GUI updates might lag. Or downright be unresponsive when the calculations are not multithreaded.
  - **Solution:** Be patient. That's it. You can monitor the console to confirm that calculations are ongoing.

## 10.2 Interpreting Warnings

- **Warning: "Invalid system matrix M..." / "Numerical instability..."**
  - **Indication:** The TMM calculation encountered potential numerical issues at specific wavelengths, possibly due to very high absorption or specific layer thickness combinations. R and T might be set to 0 for that wavelength.
  - **Impact:** Usually minor if only affecting a few wavelengths. May slightly affect integrated results like Jsc. If persistent, review layer thicknesses and optical constants.
- **Warning: "Worker Error..." / "Multiprocessing pool failed..."**
  - **Indication:** An error occurred in one of the parallel processes used for optical or generation calculations.
  - **Impact:** Results for some wavelengths or combinations might be missing or inaccurate. The calculation attempts to continue with available results. Review input parameters for potential issues.

## 10.3 Tips for Accurate Simulations

- **Accurate Optical Constants:** Use high-quality, experimentally measured $n$ and $k$ data covering the full wavelength range of interest. Ensure the file format is correct.
- **Sufficient Wavelength Resolution:** Use a small enough 'Wavelength Step' (e.g., 1-5 nm) to capture sharp spectral features or interference effects, especially for optical optimisation.

- **Realistic Recombination Parameters:** Use experimentally relevant values or physically sound estimates for SRH, Auger, and radiative recombination parameters ($J_0$, n-factors, coefficients). Use the Defect Parameter window for detailed SRH modelling if possible.
- **Reasonable Resistances:** Input realistic values for series ($R_s$) and shunt ($R_{sh}$) resistance based on device architecture and expected quality. Very low $R_{sh}$ or very high $R_s$ can significantly impact results.
- **Verify R+T+A Sum:** Check the optical plot. The R+T+A curve (green dotted line) should be close to 1 across the spectrum, indicating energy conservation in the optical model. Deviations might suggest issues with optical constants or numerical stability.
- **Start Simple:** Begin with a basic model and gradually add complexity (e.g., detailed SRH, layer mixing) to understand the impact of each parameter.

## 10.4 Frequently Asked Questions

- **Q: Can SOLEY simulate textured surfaces?**
- A: No, SOLEY's TMM assumes perfectly flat, parallel interfaces. Roughness or texturing is not directly modelled. Diffuse light simulation can approximate some effects of scattering.
- **Q: How accurate is the detailed balance model compared to drift-diffusion?**
- A: When recombination parameters are well-characterised, the detailed balance model in SOLEY can provide results (Voc, Jsc, FF, Eff) very close to drift-diffusion solvers, especially for devices not heavily limited by complex transport phenomena. However, it does not provide spatial information like band diagrams or carrier profiles.
- **Q: Can I model organic solar cells (OSCs) or perovskites?**
- A: Yes, provided you have accurate optical constants $(n, k)$ for the materials. You may have to use the layer mixing functionality. The electrical model (detailed balance + recombination) is general, but the accuracy depends on how well the chosen recombination parameters (SRH, Auger, radiative) represent the dominant loss mechanisms in those specific materials. You might need to use the custom $J_0$ feature too, for non-standard recombination models (e.g., bimolecular recombination in OSCs). But the solar cell model used is quite universal, normally.
- **Q: Why is the optimisation or batch calculation taking so long?**
- A: Be patient. Merci.

# 11 Appendix

## 11.1 List of Physical Constants Used

SOLEY uses constants from the `scipy.constants` library (based on CODATA values):

- Elementary charge ($q$): `constants.e` ($\approx 1.602 \times 10^{-19}$ C)
- Planck's constant ($h$): `constants.h` ($\approx 6.626 \times 10^{-34}$ J·s)
- Speed of light in vacuum ($c$): `constants.c` ($\approx 2.998 \times 10^{8}$ m/s)
- Boltzmann constant ($k$ or $k_B$): `constants.k` ($\approx 1.381 \times 10^{-23}$ J/K)
- Electron mass ($m_e$): `constants.m_e` ($\approx 9.109 \times 10^{-31}$ kg) - Used as $m_0$ for effective mass calculations.

## 11.2 References


- Shockley, W., & Queisser, H. J. (1961). Detailed Balance Limit of Efficiency of p-n Junction Solar Cells. *Journal of Applied Physics*, 32(3), 510–519. (Fundamental detailed balance limit)