SOLEY User Manual Version 1.5

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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 (η).

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.
- **Luminescence Spectroscopy:** NEW in v1.5 - Integrated photoluminescence (PL) and electroluminescence (EL) modelling using complete SOLEY physics for characterisation and analysis.
- **Shockley-Queisser Limit Calculator:** NEW in v1.5 - Standalone module for detailed balance analysis with customisable parameters including Auger recombination, series and shunt resistances.
- **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 What's New in Version 1.5

This release includes significant enhancements:

- **Luminescence Spectroscopy Module:** Full implementation of PL and EL calculations using actual SOLEY device physics
- **Standalone SQ Limit Calculator:** External tool for theoretical efficiency limit analysis
- **Improved Multijunction J-V Calculation:** Enhanced accuracy for 2-terminal configurations
- **Enhanced User Interface:** Streamlined workflow with better organisation of parameters
- **Performance Improvements:** Optimised calculations for faster simulations

1.4 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.
- **Luminescence:** Planck emission equations modified by device physics (quasi-Fermi level splitting, voltage-dependent recombination) to calculate realistic PL and EL spectra.

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

1.5 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 μ_n, μ_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.

1.6 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.

1.6.1 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 broad range of configurations (yes, it can still be broken if one tries hard enough).

1.6.2 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.

1.6.3 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.

1.6.4 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.

1.7 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**.

1.7.1 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.

1.7.2 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 multijunction 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.
- **Luminescence Spectroscopy:** NEW in v1.5 - Models photoluminescence and electroluminescence spectra using complete device physics, enabling characterisation analysis and defect studies.

1.7.3 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 **Optical** tab (top right):

- 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 Simulation** button located in the top left panel. 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 plot area (bottom left) 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.
- Enter the bandgap value (in eV) in the corresponding **Bandgap** entry box in the **Device Model** tab. Up to six absorbers can be defined.
- Click the **Update Bandgaps** button after entering values manually. Don't forget, seriously.

2.8 Setting Basic Device Parameters

In the **Device Model** tab (top 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.

- Use the **Injection Level** slider to adjust the intensity of the incident spectrum (simulates concentration). The label shows the equivalent power density (mW/cm^2) or concentration factor.

In the **Resistance** and **Auger** tabs:

- Input **Series (Rs)** and **Shunt (Rsh)** resistances (in Ohm·cm^2) for each defined absorber layer.
- Input **Auger coefficients** for electrons and holes for each absorber.

Other parameters like SRH recombination can be set in the **Defects** tab for more detailed modelling (see Section 6).

2.9 Running the Device Calculation

Click the **CALCULATE DEVICE PARAMS** button in the bottom right panel. 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 right:

- 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.
- 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 Sim** button in the top left panel.
- Choose a file name and location. The simulation state is saved as a `.soley` file (JSON format).
- Use the **Load Sim** button to open previously saved files. If you moved the optical spectrum 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 Stack Management - Defines the device structure and primary action buttons.
- **Top Right:** Tabbed Controls Panel - Contains organized parameter inputs (Optical, Device Model, Auger, Resistance, Defects).
- **Bottom Left:** Optical Profile Plot - Displays optical results (R, T, A).
- **Bottom Right:** Device Performance - Contains calculation buttons and results table.

3.2 Layer Stack Management Panel (Top Left)

This panel manages the layers of the solar cell stack.

- **Action Buttons:** Run Optical Simulation, Export Profile, Export Gen, Save Sim, Load Sim
- **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/Add Air Buttons:** Located below the list, used to add new layers.

3.3 Tabbed Controls Panel (Top Right)

This panel organizes parameters into logical tabs:

3.3.1 Optical Tab

Controls the optical simulation settings:

- **Wavelength Min/Max/Step:** Defines the spectral range and resolution (nm).
- **Angle:** Angle of incoming light relative to the surface normal (degrees).
- **Smoothing Controls:**
  - **Enable Curve Smoothing:** Activates/deactivates Savitzky-Golay smoothing of the calculated R, T, A data.
  - **Window Length:** Sets the filter window size (odd integer).
  - **Poly Order:** Sets the order of the polynomial used for smoothing.
- **Light Properties:**
  - **Diffuse Light:** Switches calculation mode to diffuse (hemispherical) illumination.
  - **Angle Steps:** Sets the number of discrete angles used to approximate the hemisphere.
- **Polarisation:** Selects TE, TM, or Unpolarised light.

3.3.2 Device Model Tab

Controls electrical simulation parameters:

- **Spectrum & Injection:**
  - **Load Spectrum:** Browse and select the incident solar spectrum file.
  - **Injection Level Slider:** Logarithmic slider adjusts the intensity (0.001 to 46300 suns).
- **Temperature:** Operating temperature in Kelvin.
- **Absorber Bandgaps:** Input fields for the bandgap (eV) of each absorber (1-6).
- **Update Bandgaps Button:** Applies manually entered bandgap values.

3.3.3 Auger Tab

Input fields for Auger coefficients:

- **Electrons:** Auger coefficients for electrons (e1-e6) in cm^6/s
- **Holes:** Auger coefficients for holes (h1-h6) in cm^6/s

3.3.4 Resistance Tab

Input fields for parasitic resistances:

- **Series Resistance:** Rs1-Rs6 in $Ohm \cdot cm^2$
- **Shunt Resistance:** Rsh1-Rsh6 in $Ohm \cdot cm^2$

3.3.5 Defects Tab

Controls for SRH recombination modeling:

- **Absorber Buttons (1-6):** Opens the Define Defect Profile window for each absorber.
- **Doping Type:** Dropdown to select p-type or n-type doping for each absorber.

3.4 Optical Profile Plot (Bottom Left)

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.
- Grid lines aid visualisation.

3.5 Device Performance Panel (Bottom Right)

Controls electrical calculations and displays results:

- **Action Buttons:**
  - **CALCULATE DEVICE PARAMS:** Main calculation button (blue, bold)
  - **J-V Curves:** Opens J-V plotting window (green)
  - **Luminescence:** Opens luminescence spectroscopy window (purple) - NEW in v1.5
  - **SQ Limit:** Opens Shockley-Queisser limit calculator (brown) - NEW in v1.5
  - **Batch Calc:** Opens batch calculation window (pink)
  - **Optimise Stack:** Opens layer optimisation window (cyan)
  - **SQ Step:** Calculate device with SQ radiative limit only (teal)
  - **Clear Table:** Clears the results table
- **Results Table:** Displays calculated device parameters in a scrollable text area with fixed-width font for alignment.

3.6 Buttons and Menu Actions (Summary)

Key action buttons are distributed across the panels as described above. 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 ϵ_{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 ϵ_1, ϵ_2 are their respective complex dielectric permittivities ($\epsilon = (n + ik)^2$). SOLEY solves this equation iteratively at each wavelength to find ϵ_{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:

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

  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).

- **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 σ, 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 Luminescence Spectroscopy Model (NEW in v1.5)

SOLEY v1.5 introduces comprehensive luminescence modelling that uses the complete device physics.

4.4.1 Theoretical Framework

Luminescence emission from a semiconductor is governed by the generalized Planck equation modified by the quasi-Fermi level splitting:

$$\Phi_{em}(E) = \frac{2\pi}{h^3 c^2} \cdot E^2 \cdot A(E) \cdot \frac{1}{e^{(E-\Delta\mu)/kT} - 1} \tag{22}$$

where Φ_{em} is the emitted photon flux, E is the photon energy, $A(E)$ is the absorptivity (from TMM), and $\Delta\mu$ is the quasi-Fermi level splitting.

4.4.2 Photoluminescence (PL)

For photoluminescence, SOLEY:

- Calculates absorbed excitation power at the specified wavelength using TMM
- Determines the quasi-Fermi splitting using `detailed_balance_sq_limit_single()`
- Supports two operating modes:
  - **Open circuit:** Full quasi-Fermi splitting from photogeneration
  - **Fixed voltage:** Constrains splitting to applied bias (for voltage-dependent studies)
- Computes emission spectrum accounting for reabsorption (using step function or detailed TMM absorptivity)

4.4.3 Electroluminescence (EL)

For electroluminescence, SOLEY:

- Uses `compute_jv_curve_for_absorber()` to determine device physics at applied voltage
- Calculates quasi-Fermi splitting from the injected current
- Applies internal quantum efficiency factor
- Computes emission spectrum with complete device physics (recombination, resistances, etc.)

4.4.4 Advanced Features

- **Absorptivity Options:**
  - Step function: Simplified model assuming unity absorption above bandgap
  - Detailed TMM: Uses actual optical calculations with reabsorption effects
- **Angular Integration:** For emitted light escaping the device, uses diffuse emission or specified extraction angle
- **Multi-absorber Support:** Can calculate luminescence for each absorber independently
- **Logarithmic/Linear Scale:** Flexible plotting for different intensity ranges

4.5 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 smoothing functionality and numerical stability enhancements were added.

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 optical profile plot.

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:

$$G(x, \lambda) \propto \alpha(\lambda) \cdot I(x, \lambda) \tag{23}$$

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):

$$G_{tot}(x) = \int_{\lambda_{min}}^{\lambda_{max}} \frac{\alpha(\lambda) I(x, \lambda)}{I_{in}(\lambda)} \Phi_{in}(\lambda) d\lambda \tag{24}$$

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 θ.
- 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 θ (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 is particularly problematic when using a glass substrate or superstrate, for example.

- If 'Enable Curve 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 'Poly 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.

5.7 Exporting Optical Profile and Generation Data

- **Export Profile:** Saves the currently plotted R, T, and layer-specific A values (after any smoothing) versus wavelength to a CSV file.
- **Export Gen:** 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:

$$J = J_{ph} - J_{rec}(V_j) - \frac{V_j}{R_{sh}} \quad \text{where } V_j = V + J \cdot R_s \tag{25}$$

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.

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:

$$FF = \frac{V_{mp} \times J_{mp}}{V_{oc} \times J_{sc}} \tag{26}$$

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

$$\eta = \frac{P_{max}}{P_{in}} = \frac{V_{oc} \times J_{sc} \times FF}{P_{in}} \tag{27}$$

  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 parameter scales the radiative recombination current $J_{0,rad}$. The default value (1.09×10^{-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), σ_n (capture cross-section), v_{th} (thermal velocity), N_c, N_v, N_{dop}, V_{bi}, ϵ (permittivity) for the absorber, and S_p (interface recombination velocity), $N_{c,adj}$, $N_{dop,adj}$, θ 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 Scaffidi 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 **J-V Curves** 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 (η_{MJ}) are calculated based on these combined $J_{sc,MJ}$ and $V_{oc,MJ}$ values, using an improved voltage-mapping approach for the combined J-V curve.
- 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:

$$J_{\mathrm{MJ}}(V) = J_1(V_1) = J_2(V_2) = \ldots = J_n(V_n) \tag{28}$$

$$V_{\mathrm{MJ}} = \sum_{i=1}^{n} V_i \tag{29}$$

where J_{MJ} is the multijunction current density, V_{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_{common} from a negative value (typically $-0.5 \times J_{\text{sc,min}}$) to slightly above the minimum J_{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 $V_{\text{MJ},j} = \sum_{i=1}^{n} V_{i,j}$
3. This yields the multijunction J-V relationship as a set of points $(V_{\text{MJ},j}, J_j)$

7.3 Mathematical Formulation

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

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

where J_{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_{sh} is the shunt resistance.

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

$$f(V, J) = J - J_{\text{sc}} + J_0 \left(\exp\left(\frac{q(V + JR_s)}{nkT} \right) - 1 \right) + \frac{V + JR_s}{R_{\text{sh}}} = 0 \tag{31}$$

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:

$$FF_{\text{MJ}} = \frac{P_{\text{max}}}{J_{\text{sc,MJ}} \times V_{\text{oc,MJ}}} = \frac{J_{\text{mp}} \times V_{\text{mp}}}{J_{\text{sc,MJ}} \times V_{\text{oc,MJ}}} \tag{32}$$

where J_{mp} and V_{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_{sc}, V_{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. However, 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.

8 Luminescence Spectroscopy Module (NEW in v1.5)

8.1 Overview

The Luminescence Spectroscopy module provides comprehensive photoluminescence (PL) and electroluminescence (EL) modeling integrated directly with SOLEY's device physics. Unlike simplified models, this implementation uses the complete TMM optical calculations and detailed balance framework to produce physically accurate spectra.

8.2 Accessing the Module

- Click the **Luminescence** button in the Device Performance panel (purple button)
- Prerequisites: Optical calculations must be completed first (TMM data required)
- At least one absorber layer must be defined

8.3 Interface Layout

The luminescence window is divided into two main panels:

- **Left Panel:** Controls and parameters (scrollable)
- **Right Panel:** Spectrum plot with dual axes (energy and wavelength)

8.4 Photoluminescence (PL) Parameters

8.4.1 Basic PL Settings

- **Enable PL:** Checkbox to include PL in calculations
- **Excitation (nm):** Wavelength of the excitation laser/source
- **Power (mW/cm²):** Excitation power density
- **Voltage Mode:**
  - *Open circuit:* Full quasi-Fermi splitting (uses `detailed_balance_sq_limit_single()`)
  - *Fixed V:* Constrains splitting to applied bias for voltage-dependent PL studies

8.4.2 PL Physical Model

The PL spectrum is calculated using:

$$\Phi_{PL}(E) = \frac{2\pi}{h^3c^2} \cdot E^2 \cdot A(E) \cdot \frac{1}{e^{(E-\Delta\mu_{PL})/kT} - 1} \tag{33}$$

where:

- $\Delta\mu_{PL}$ is the quasi-Fermi splitting from photogeneration
- $A(E)$ is the absorptivity from TMM (accounting for reabsorption)
- Excitation power determines carrier generation and splitting

8.5 Electroluminescence (EL) Parameters

8.5.1 Basic EL Settings

- **Enable EL:** Checkbox to include EL in calculations
- **Applied voltage (V):** Forward bias voltage for injection
- **Internal efficiency :** Quantum efficiency factor (0-1)

8.5.2 EL Physical Model

The EL spectrum is calculated using:

$$\Phi_{EL}(E) = \eta_{int} \cdot \frac{2\pi}{h^3 c^2} \cdot E^2 \cdot A(E) \cdot \frac{1}{e^{(E-qV)/kT} - 1} \tag{34}$$

where:

- Uses `compute_jv_curve_for_absorber()` for device physics at applied voltage
- Accounts for series resistance, recombination, and injection effects
- Internal efficiency factor scales the emission intensity

8.6 Advanced Options

8.6.1 Absorptivity Model Selection

- **Use step function:** Simplified model assuming A(E) = 1 for E ¿ Eg, A(E) = 0 otherwise
- **Use detailed TMM:** Full optical calculation with wavelength-dependent absorptivity and reabsorption effects (recommended for accurate spectra)

8.6.2 Multi-Absorber Support

- Select which absorber layer to calculate luminescence for
- Each absorber can have different PL and EL characteristics
- Useful for studying individual subcells in multijunction devices

8.6.3 Plot Options

- **Y-axis Scale:** Toggle between logarithmic (default) and linear scale
- **Dual Axes:** Bottom axis shows photon energy (eV), top axis shows wavelength (nm)
- **Update Visibility:** Show/hide PL or EL curves independently

8.7 Results Display

The results textbox shows calculated parameters:

- Quasi-Fermi level splitting ($\Delta\mu$) in eV
- Implied open-circuit voltage from splitting
- Peak emission wavelength/energy
- Integrated photon flux
- Operating conditions (temperature, voltage, excitation power)

8.8 Exporting Data

8.8.1 Export Data (CSV)

Creates a CSV file containing:

- Energy (eV) and wavelength (nm) columns
- PL photon flux (photons/m²/s/eV) if enabled
- EL photon flux (photons/m²/s/eV) if enabled
- Metadata header with calculation parameters

8.8.2 Export Plot

Saves the current plot as a high-resolution image file (PNG, PDF, or SVG format).

8.9 Typical Workflow

8.9.1 Basic PL Measurement Simulation

1. Complete optical TMM simulation in main SOLEY window
2. Define absorber layers and bandgaps
3. Open Luminescence window
4. Set excitation wavelength (e.g., 532 nm for green laser)
5. Set excitation power (typical: 1-100 mW/cm²)
6. Enable "Use detailed TMM absorptivity" for accuracy
7. Click "Calculate Spectra"
8. Analyze PL peak position and shape

8.9.2 Voltage-Dependent PL

1. Follow steps 1-6 from basic PL
2. Switch to "Fixed V" mode
3. Enter desired voltage
4. Calculate and observe how spectrum shifts with voltage
5. Repeat for multiple voltages to study recombination dynamics

8.9.3 EL Characterisation

1. Ensure device parameters are properly defined (resistances, recombination)
2. Open Luminescence window
3. Enable EL, disable PL
4. Set applied forward bias voltage
5. Adjust internal efficiency if known (default 1.0)
6. Calculate to see emission under electrical injection

8.9.4 Combined PL and EL Analysis

1. Enable both PL and EL
2. Set appropriate parameters for each
3. Calculate to compare photo- and electro-generated emission
4. Use logarithmic scale to see both spectra if intensities differ greatly
5. Export data for quantitative comparison

8.10 Physical Interpretation

8.10.1 PL Peak Position

- Typically near the bandgap energy
- Red-shift indicates band-gap renormalisation or Stokes shift
- Blue-shift possible with high excitation (band-filling effects)
- Shape depends on absorptivity profile and reabsorption

8.10.2 PL Intensity

- Higher intensity indicates better material quality (lower non-radiative recombination)
- Absolute intensity depends on excitation power and extraction efficiency
- Ratio of PL to excitation power gives external quantum efficiency information

8.10.3 EL Characteristics

- EL onset voltage near open-circuit voltage
- Peak position should match PL peak (same radiative transitions)
- EL efficiency decreases with increasing non-radiative recombination
- Series resistance causes voltage shift between injection and emission

8.11 Troubleshooting

8.11.1 No PL/EL Signal

- Check that optical calculations completed successfully
- Verify absorber layer is defined with correct bandgap
- For PL: excitation wavelength must be above bandgap
- For EL: applied voltage must be sufficient for injection
- Check if absorptivity is being calculated (Calc A checkbox)

8.11.2 Unrealistic Spectra

- Try "detailed TMM absorptivity" instead of step function
- Verify TMM wavelength range covers emission region
- Check temperature setting (affects spectral shape)
- For EL: verify device physics parameters are realistic

8.11.3 Intensity Issues

- Use logarithmic scale for wide intensity ranges
- For PL: higher excitation power increases signal
- For EL: internal efficiency factor scales output
- Absolute intensities depend on extraction geometry (not explicitly modeled)

9 Shockley-Queisser Limit Calculator (NEW in v1.5)

9.1 Overview

The SQ Limit Calculator is a standalone tool for exploring theoretical efficiency limits of solar cells. It extends the classic Shockley-Queisser framework to include Auger recombination and parasitic resistances, allowing more realistic limit calculations.

9.2 Accessing the Calculator

- Click the **SQ Limit** button in the Device Performance panel (brown button)
- Opens as an independent window
- Does not require optical calculations (uses direct spectral integration)

9.3 Interface Layout

The SQ Limit window contains:

- **Top Section:** Spectrum selection and loading
- **Left Panel:** Parameter controls organized in collapsible sections
- **Right Panel:** Results plot showing efficiency vs bandgap
- **Bottom Section:** Results table with numerical values

9.4 Spectrum Selection

- **Load Spectrum:** Select incident spectrum file (same format as main SOLEY)
- Spectrum must be in wavelength-power format (nm, W/m²/nm)
- Automatically converts to energy-power format internally
- Displays spectrum filename in label after loading

9.5 Basic Parameters

9.5.1 Bandgap Range

- **E_g_min (eV):** Minimum bandgap for sweep (default 0.5)
- **E_g_max (eV):** Maximum bandgap for sweep (default 4.0)
- **E_g_step (eV):** Step size for bandgap sweep (default 0.01)
- Finer steps give smoother curves but take longer to calculate

9.5.2 Operating Conditions

- **Temperature (K):** Cell operating temperature (default 300)
- **Injection Factor:** Light concentration (logarithmic slider)
  - Range: 0.001 to 46300 suns
  - Default: 1.0 (standard 1-sun AM1.5G)
  - Displays equivalent power density in mW/cm²

9.6 Parasitic Resistances

9.6.1 Series Resistance

- **R_s (·cm²):** Lumped series resistance (default 0)
- Reduces output voltage and fill factor
- Typical values: 0.1-10 ·cm² for real devices
- Logarithmic slider for wide range access

9.6.2 Shunt Resistance

- **R_sh (·cm²):** Lumped shunt resistance (default 10000)
- Provides leakage current path
- Typical values: 1000-100000 ·cm² for good devices
- Logarithmic slider for wide range access

9.7 Auger Recombination (Optional)

9.7.1 Enable/Disable Auger

- Checkbox to include Auger recombination in calculations
- When disabled, uses purely radiative limit
- When enabled, requires additional parameters

9.7.2 Auger Parameters

- **C_A_n (cm/s):** Electron Auger coefficient
- **C_A_p (cm/s):** Hole Auger coefficient
- **Thickness (m):** Active layer thickness
- **m_e_eff (m):** Effective electron mass
- **m_h_eff (m):** Effective hole mass

These parameters determine the Auger saturation current:

$$J_{0,Auger} = q \cdot d \cdot C_A \cdot N_{dop}^2 \cdot n_i \tag{35}$$

9.8 Calculation and Results

9.8.1 Running Calculations

- Click **Calculate SQ Limit** button
- Sweeps through specified bandgap range
- For each bandgap:
  - Calculates ideal Jsc from spectrum
  - Calculates J0_rad from detailed balance
  - Includes J0_Auger if enabled
  - Solves for Voc, FF, and efficiency considering resistances
- Progress shown in status messages

9.8.2 Results Plot

Displays efficiency (

- Peak efficiency and corresponding optimal bandgap
- Effect of non-radiative losses (if Auger enabled)
- Impact of resistances on peak efficiency
- Shape of efficiency curve for material selection

9.8.3 Results Table

Shows detailed parameters at optimal bandgap:

- Optimal E_g (eV)
- Maximum efficiency (
- Jsc (mA/cm²) at optimal gap
- Voc (V) at optimal gap
- Fill Factor (
- J0_rad and J0_Auger (if applicable)

9.9 Exporting Results

9.9.1 Export Plot

Saves the efficiency vs bandgap plot as an image file.

9.9.2 Export Data

Creates CSV file with columns:

- Bandgap (eV)
- Efficiency (
- Jsc (mA/cm²)
- Voc (V)
- FF (
- J0_rad (A/cm²)
- J0_Auger (A/cm²) if enabled

9.10 Typical Use Cases

9.10.1 Material Selection

1. Load appropriate spectrum (e.g., AM1.5G for terrestrial)
2. Set realistic temperature (300K typical)
3. Keep resistances at zero for ideal limit
4. Disable Auger for fundamental Shockley-Queisser limit
5. Calculate to find optimal bandgap for given spectrum
6. Compare with candidate material bandgaps

9.10.2 Loss Mechanism Analysis

1. Start with ideal case (no Auger, no resistances)
2. Note peak efficiency
3. Enable Auger with material-specific coefficients
4. Observe efficiency reduction
5. Add realistic resistances
6. Quantify each loss mechanism's impact

9.10.3 Concentration Effects

1. Set up with realistic Auger parameters
2. Calculate at 1 sun (default)
3. Increase injection factor (concentration)
4. Observe how Voc increases (logarithmically)
5. Note that Auger losses increase with concentration
6. Find optimal concentration considering both effects

9.10.4 Multijunction Design

1. Calculate single-junction limit for reference
2. For tandem: identify two peak regions
3. Top cell: higher bandgap (around first peak)
4. Bottom cell: lower bandgap (around second peak)
5. Sum of subcell efficiencies gives tandem limit estimate
6. Consider current-matching requirements

9.11 Understanding the Physics

9.11.1 The Shockley-Queisser Limit

The fundamental efficiency limit arises from:

- **Thermalisation:** Photons above Eg lose excess energy as heat
- **Sub-bandgap loss:** Photons below Eg are not absorbed
- **Radiative recombination:** Unavoidable in thermal equilibrium
- **Entropy:** Conversion of high-energy photons to voltage-limited work

9.11.2 Effect of Auger Recombination

- Three-particle process: scales as n^3 or p^3
- Becomes dominant in narrow-gap materials
- Particularly important at high concentrations
- Reduces Voc by providing additional recombination path
- More severe in highly doped materials

9.11.3 Impact of Resistances

- **Series resistance:** Mainly reduces FF, slight Voc loss
  - Voltage drop: $V_{loss} = J \cdot R_s$
  - Maximum at maximum power point
  - More severe at high current densities
- **Shunt resistance:** Reduces Voc and FF
  - Leakage current: $J_{leak} = V/R_{sh}$
  - Most severe at low voltages
  - Limits Voc if too low

9.12 Advanced Features

9.12.1 Custom Spectrum Analysis

- Load custom spectrum files for specific applications
- Indoor lighting: different optimal bandgap than solar
- Space: AM0 spectrum gives different limits
- Monochromatic: narrow peak, very application-specific

9.12.2 Temperature Studies

- Vary temperature to see thermal effects
- Higher T: lower Voc (entropy loss)
- Lower T: higher efficiency (reduced recombination)
- Important for space applications or hot-climate deployment

9.12.3 Material Comparison

- Calculate with different Auger coefficients
- Compare direct vs indirect bandgap materials
- Assess thickness requirements (for Auger calculation)
- Evaluate different doping levels

9.13 Limitations and Considerations

- Assumes perfect absorption above bandgap (no reflection/transmission losses)
- Does not account for interface recombination explicitly
- Auger model uses simple bulk approximation
- Resistances are lumped parameters (no spatial distribution)
- Temperature is uniform (no gradients)
- Ideal current collection (no transport losses)

For more realistic device modeling including these effects, use the main SOLEY interface with full TMM and defect modeling.

10 Advanced Features

SOLEY includes features for optimisation and systematic parameter exploration.

10.1 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 **Optimise Stack** button.
- A window appears listing all layers in the stack.
- **Setting Parameters:** For each layer you want to optimise:
  - Check the **Optimise** 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 Optimisation**. 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.

10.2 Batch Calculations

This feature allows automated simulation runs while systematically varying one or more parameters.

- Access via the **Batch Calc** 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.

10.3 Saving and Loading Simulation States

- **Save Sim:** 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, injection factor, resistances, Auger coefficients, bandgaps, SRH defect parameters).

  The data is saved in a single `.soley` file (JSON format).
- **Load Sim:** 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.

10.4 Simulating Diffuse Light Effects

- Check the **Diffuse Light** box in the Optical tab.
- 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 Simulation** 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 Gen** 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.

11 File Formats

SOLEY uses specific file formats for input and output data.

11.1 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
```

11.2 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
```

11.3 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, injection factor, resistances, Auger coefficients, 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.

11.4 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.
- **Luminescence Data:** Columns for Energy (eV), Wavelength (nm), PL flux, EL flux (photons/m^2/s/eV).

12 Troubleshooting and FAQ

This section addresses common issues and questions.

12.1 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 Model tab.
  - **Solution:** Click 'Load Spectrum' 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 Stack 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 be unresponsive when calculations are not multithreaded.
  - **Solution:** Be patient. Monitor the console to confirm that calculations are ongoing.
- **Luminescence window shows no signal**
  - **Cause:** TMM calculations not completed, or absorber not properly defined.
  - **Solution:** Run optical calculations first, ensure absorber checkbox is ticked and bandgap is set.

12.2 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.

12.3 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 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.

12.4 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 for non-standard recombination models (e.g., bimolecular recombination in OSCs).
- **Q: What's the difference between the luminescence module and just calculating J-V?**
- A: The luminescence module calculates the emitted photon spectrum based on device physics, which is useful for material characterisation and understanding recombination dynamics. J-V curves show electrical performance. Both use the same underlying physics but provide different perspectives.
- **Q: Should I use the SQ Limit Calculator or the main SOLEY interface?**
- A: Use the SQ Limit Calculator for theoretical limit studies and material selection. Use the main SOLEY interface for realistic device modeling with actual layer stacks, optical effects, and detailed recombination mechanisms.
- **Q: Why is optimisation or batch calculation taking so long?**
- A: Be patient. The number of calculations scales exponentially with the number of varied parameters and steps.
- **Q: Can I import optical data from ellipsometry directly?**
- A: SOLEY requires data in the simple three-column format (wavelength, n, k). Most ellipsometry software can export to this format. Ensure wavelengths are in nm and sorted in ascending order.

13 Version History

13.1 Version 1.5 (Current)

- Added Luminescence Spectroscopy module (PL and EL)
- Added standalone Shockley-Queisser Limit Calculator
- Improved multijunction J-V calculation methodology

- Enhanced user interface with better organisation
- Performance optimisations for faster calculations
- Bug fixes and stability improvements

13.2 Version 1.0.1 (Previous)

- Initial public release
- Core TMM optical calculations
- Detailed balance device modeling
- SRH defect modeling framework
- Batch calculations and optimisation
- Layer mixing (Bruggeman EMA)

14 Appendix

14.1 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.

14.2 Acknowledgments

SOLEY development has benefited from extensive testing and feedback from the photovoltaics research community. The Scaffidi formulation for SRH recombination is based on work by Cuevas and colleagues.

14.3 Contact and Support

For questions, bug reports, or feature requests:

- Email: zacharie.jehl@upc.edu
- Include "SOLEY" in the subject line
- Provide version number (1.5) and detailed description of issue

14.4 Citing SOLEY

If you use SOLEY in your research, please cite:

- Software: SOLEY v1.5 (Solar Cell Optics and Electrics), Zacharie Jehl Li-Kao, 2025
- Methodology papers (to be published)

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