Solar cell simulation

Below is a summary of the PN union model and also a guide to the algorithm used to perform the simulations shown in this repository. The equations were taken from the work of the researcher Arturo Morales Acevedo and collaborators, who provides an explanation of the model in https://www.sciencedirect.com/science/article/pii/S1665642317300950.

1. PN unión model

The simulation consists in determining the total current density produced by the cell, using next expressions and taking into account the application of an external voltage. The analytical solution is subject to two overlapping scenarios in the general solution: when the cell is in darkness (J_{dark}) and when it is in illumination (J_{ph}). Thus, the current density of the cell (J_{cell}) is expressed as:

$$J_{cell}(V) = J_{ph}(V) - J_{dark}(V) \qquad (3.4)$$

The current densities in lighting and darkness are given by:

$$J_{ph}(V) = \int_{\lambda min}^{\lambda max} \left[J_n^{'}(\lambda) + J_p^{'}(\lambda) + J_{scr}^{'}(\lambda) \right] d\lambda \qquad (3.5)$$

$$J_{dark}(V) = J_0\left(e^{\frac{qV}{k_B T}} - 1\right) + J_{00}\left(e^{\frac{qV}{2k_B T}} - 1\right) \qquad (3.6)$$

In both equations the dependence with respect to voltage V is indicated, which is necessary for the construction of the J vs V diagrams that characterize the behavior of a solar cell. There are multiple variables involved. In equation 3.5, the dependence of J_{ph} (photocurrent density) with respect to three terms is observed: the first two, Jn 'and Jp' are the current densities for electrons and holes due to diffusion in the quasi - neutrality; the third term Jscr 'is the current density due to entrainment in the space-charge region. Equation 3.6, seeks to obtain the J_{dark} dark current density using two relevant terms: the first, J_0 is the dark saturation current due to diffusion and the second, J_{00} the dark saturation current due to generation - recombination in the space-cargo region. Each of these stated values are calculated from other expressions, shown below.

- **Photocurrent density limited by ambipolar diffusion**

$$J_p^{'}(\lambda) = \frac{qN_0(1-R)T\alpha_1 L_p}{\left(\alpha_1^2 L_p^2 - 1\right)}\left(\frac{\frac{S_p L_p}{D_p} + \alpha_1 L_p - e^{-\alpha_1\left(W_n - x_n\right)}\left(\frac{S_p L_p}{D_p}\cosh\left(\frac{W_n - x_n}{L_p}\right) + \sinh\left(\frac{W_n - x_n}{L_p}\right)\right)}{\frac{S_p L_p}{D_p}\sinh\left(\frac{W_n - x_n}{L_p}\right) + \cosh\left(\frac{W_n - x_n}{L_p}\right)} - \alpha_1 L_p e^{-\alpha_1\left(W_n - x_n\right)}\right) \qquad (3.7)$$

$$J_n^{'}(\lambda) = \frac{qN_0(1-R)T\alpha_2 L_n}{\left(\alpha_2^2 L_n^2 - 1\right)} e^{\left(-\alpha_1 W_n - \alpha_2 x_p\right)}\left(\alpha_2 L_n - \frac{\frac{S_n L_n}{D_n}\left(\cosh\left(\frac{W_p - x_p}{L_n}\right) - e^{-\alpha_2\left(W_p - x_p\right)}\right) + \sinh\left(\frac{W_p - x_p}{L_n}\right) + \alpha_2 L_n e^{-\alpha_2\left(W_p - x_p\right)}}{\frac{S_n L_n}{D_n}\sinh\left(\frac{W_p - x_p}{L_n}\right) + \cosh\left(\frac{W_p - x_p}{L_n}\right)}\right) \qquad (3.8)$$

- **Photocurrent density due to drift in the space-charge region**

$$J'_{scr}(\lambda) = qN_0(1 - R)Te^{-\alpha_1(W_n - x_n)}\left(\left(1 - e^{-\alpha_1 x_n}\right) + e^{-\alpha_1 x_n}\left(1 - e^{-\alpha_2 x_p}\right)\right) \quad (3.9)$$

- **Dark saturation currents**

$$J_0(V) = J_{0p}(V) + J_{0n}(V) \quad (3.10)$$

$$J_{00}(V) = q\left(\frac{x_n n_{i,n}}{\tau_p} + \frac{x_p n_{i,p}}{\tau_n}\right) \quad (3.11)$$

$$J_{0p} = \frac{qD_p p_0}{L_p}\left(\frac{\frac{S_p L_p}{D_p}\cosh\frac{w_n - x_n}{L_p} + \sinh\frac{w_n - x_n}{L_p}}{\frac{S_p L_p}{D_p}sinh\frac{w_n - x_n}{L_p} + cosh\frac{w_n - x_n}{L_p}}\right) \quad (3.12.a)$$

$$J_{0n} = \frac{qD_n n_0}{L_n}\left(\frac{\frac{S_n L_n}{D_n}cosh\frac{w_p - x_p}{L_n} + \sinh\frac{w_p - x_p}{L_n}}{\frac{S_n L_n}{D_n}sinh\frac{w_p - x_p}{L_n} + \cosh\frac{w_p - x_p}{L_n}}\right) \quad (3.12.b)$$

- **Depletion region**

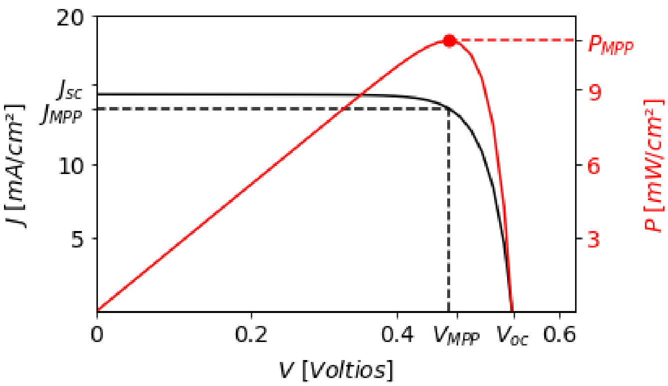
$$x_p(V) = \left(\frac{2\varepsilon_p \varepsilon_n N_d\left(V_{bi} - V\right)}{qN_a\left(\varepsilon_n N_d + \varepsilon_p N_a\right)}\right)^{\frac{1}{2}}$$

$$x_n(V) = \left(\frac{2\varepsilon_p \varepsilon_n N_a\left(V_{bi} - V\right)}{qN_d\left(\varepsilon_n N_d + \varepsilon_p N_a\right)}\right)^{\frac{1}{2}}$$

- **Built-in potential**

$$V_{bi} = \frac{\Delta E_c - \Delta E_v}{2} + k_B T \ln ln\left(\frac{N_a N_d}{n_{i,p} n_{i,n}}\right) + \frac{k_b T}{2}\ln ln\left(\frac{N_{c,p} N_{v,n}}{n_{c,n} n_{v,p}}\right) \quad (3.14)$$

Replacing the properties or values of the materials in the equations previously shown, in addition to carrying out the necessary numerical integration processes. It is possible to determine the current produced (J_{cell}). To construct the J-V curve, the described models must be simulated, using different voltage values.



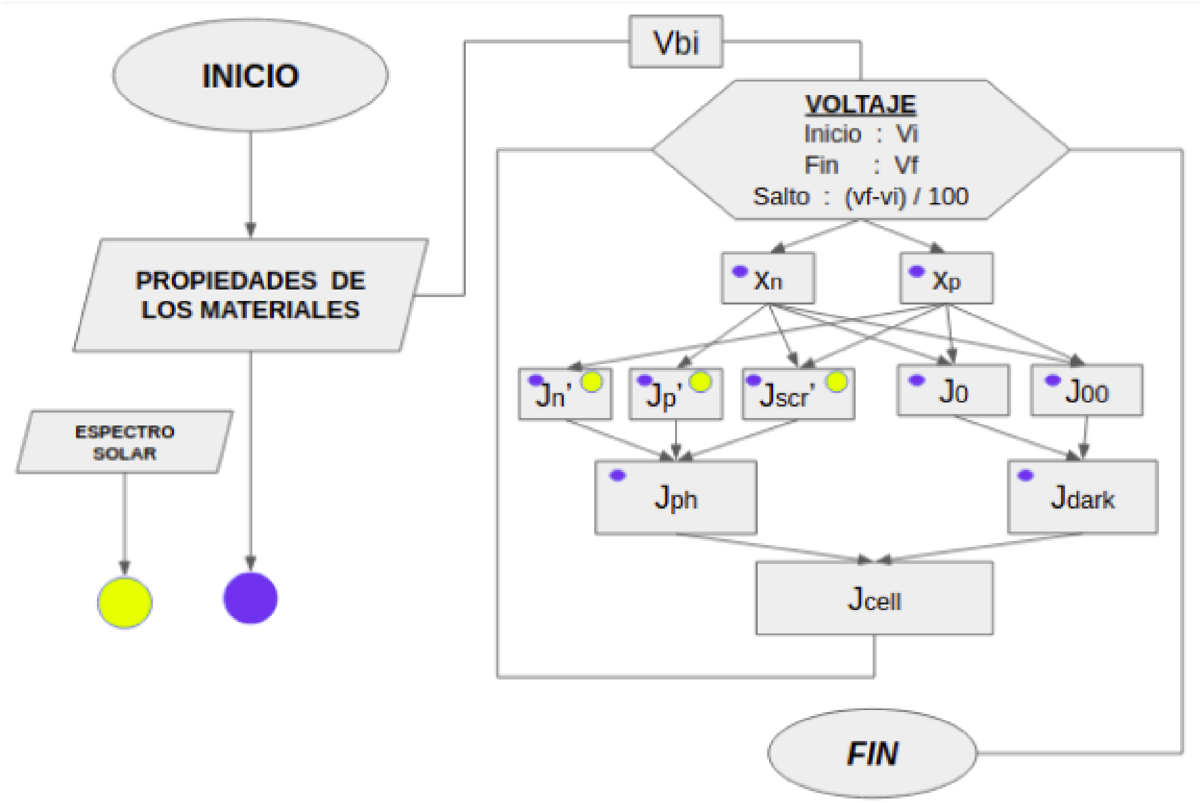
After obtaining the pairs (J, V) it is possible to determine the other variables of interest that characterize the behavior of the cell, such as the power density (P), the open circuit voltage (V_{oc}), the current density in short circuit (J_{sc}), fill factor (FF) and efficiency (η).

$$P_{MPP} = J_{MPP} V_{MPP} \qquad (3.18)$$

$$FF = \frac{J_{MPP} V_{MPP}}{J_{sc} V_{oc}} \qquad (3.19)$$

$$\eta = \frac{J_{sc} V_{oc} FF}{P_{Inc}} \qquad (3.20)$$

2. Algorithm



The functions shown in the flow chart are described below, along with their respective input and output values.

- **Built-in Potential V_{bi}** *(equation 3.14).*
  Input: ΔE_c, ΔE_v, N_a, N_d, n_{in}, n_{ip}, N_{cp}, N_{cn}, N_{vc}, N_{vn}.
  Output: V_{bi}.

  The ΔEc, ΔEv values are obtained from Anderson's rule, using the electron affinity values (χ) and the band gap (E_g) of each of the materials.

- **Depletion Region x_n y x_p** *(equations 3.13.a and 3.13.b).*
  Input: V_{bi}, V, ε_p, ε_p, N_a, N_d.
  Output: x_n, x_p.

The calculation of the photocurrent must take into account that the values J_n', J_p' and J_{scr}' are variables that correspond to the derivatives of current densities and their values depend on the wavelength. Then, a set of values is obtained as a function of λ.

- **Photocurrent J_p'** *(equation 3.7)*.
  Input: x_n, W_n, L_p, S_p, D_p, α_1, R, T, N_0.
  Output: list J_p'

- **Photocurrent J_n'** *(equation 3.8).*
  Input: x_p, W_n, W_p, L_n, S_n, D_n, α_1, α_2, N_0.
  Output: list J_n'.

- **Photocurrent J_{scr}'** *(equation 3.9).*
  Input: x_n, x_p, W_n, α_1, α_2, R, N_0.

Output: list J_{scr}'.

- **Photocurrent J_{ph}** *(equation 3.5).*
  Input: J_n', J_p', J_{scr}'.
  Output: J_{ph}.

  The lists of values provided in the input are integrated numerically using the trapezoidal method.

For the current density functions in the dark, the values J_0 and J_{00} are initially calculated. The J_0 value requires two additional functions to perform its calculation.

- **Saturation current density J_0.**
  - Function J_{0p} *(equation 3.12.a).*
    Input: $S_p, L_p, D_p, p_0, x_n, w_n$.
    Output: J_{0n}.
  - Function J_{0n} *(equation 3.12.b).*
    Input: $S_n, L_n, D_n, n_0, x_p, w_p$.
    Output: J_{0n}.
  - Function J_0 *(equation 3.10).*
    Input: J_{0n}, J_{0p}, V.
    Output: J_0.

- **Saturation current density J_{00}** *(equation 3.11).*
  Input: $x_n, x_p, n_{in}, n_{ip}, \tau_p, \tau_n$.
  Output: J_{00}.

- **Dark current density J_{dark}** *(equation 3.6).*
  Input: V, J_0, J_{00}.
  Output: J_{dark}.