PVLimits: PV thermodynamic limit calculator

Documentation

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1 Introduction and tool summary

PVLimits software calculates the thermodynamic performance limits of single-junction (SJ) and multi-junction (MJ) solar cells. The user may choose the input spectrum (e.g., AM1.5G or Blackbody, distance from the Sun, concentration, etc.) and specify the parameters of the solar cell (temperature, bandgap, number of subcells in MJ cell etc.).

The calculations are based on detailed particle balance in the radiative limit: the absorbed solar photon flux (R_{in}) is balanced by radiative recombination (R_{rad}) and the carrier collection (electrical current, J), as follows:

$$R_{in} = \frac{J(V)}{q} + R_{rad}(V).$$

Here, R_{in} (i.e., absorption flux) depends on the temperature of the 'Sun', the bandgap (E_g) of the solar cell, and its distance from the Sun. The radiative recombination $R_{rad}(V)$ depends on the temperature of the device, E_g and bias V. See refs. [1]–[5] for more details.

PVLimits has options to calculate the following:

1. Single junction PV:
    a. J-V for a single bandgap
    b. Eg-sweep: PV output parameters as a function of bandgap (Eg)
2. Multi-junction PV:
    a. J-V for a given number of subcells (N). The bandgaps are optimized accordingly
    b. N-sweep: PV output parameters as a function of number of subcells (N).

The usage of the tool is explained in the following sections.

2 Using the tool

2.1 Input

There are three parts in the input panel (see fig-1):

1. Simulation setup
2. PV inputs (simulation specific inputs)
3. Spectral input

We will discuss these three input parts in the following subsections.

2.1.1 Simulation setup

There are four simulation options as mentioned earlier:

1. Single junction PV:
    a. J-V characteristics for a single bandgap
    b. Eg-sweep: PV output parameters as a function of bandgap (Eg)
2. Multi-junction PV:
    a. J-V characteristics for a given number of subcells (N). The bandgaps are optimized accordingly
    b. N-sweep: PV output parameters as a function of number of subcells (N).

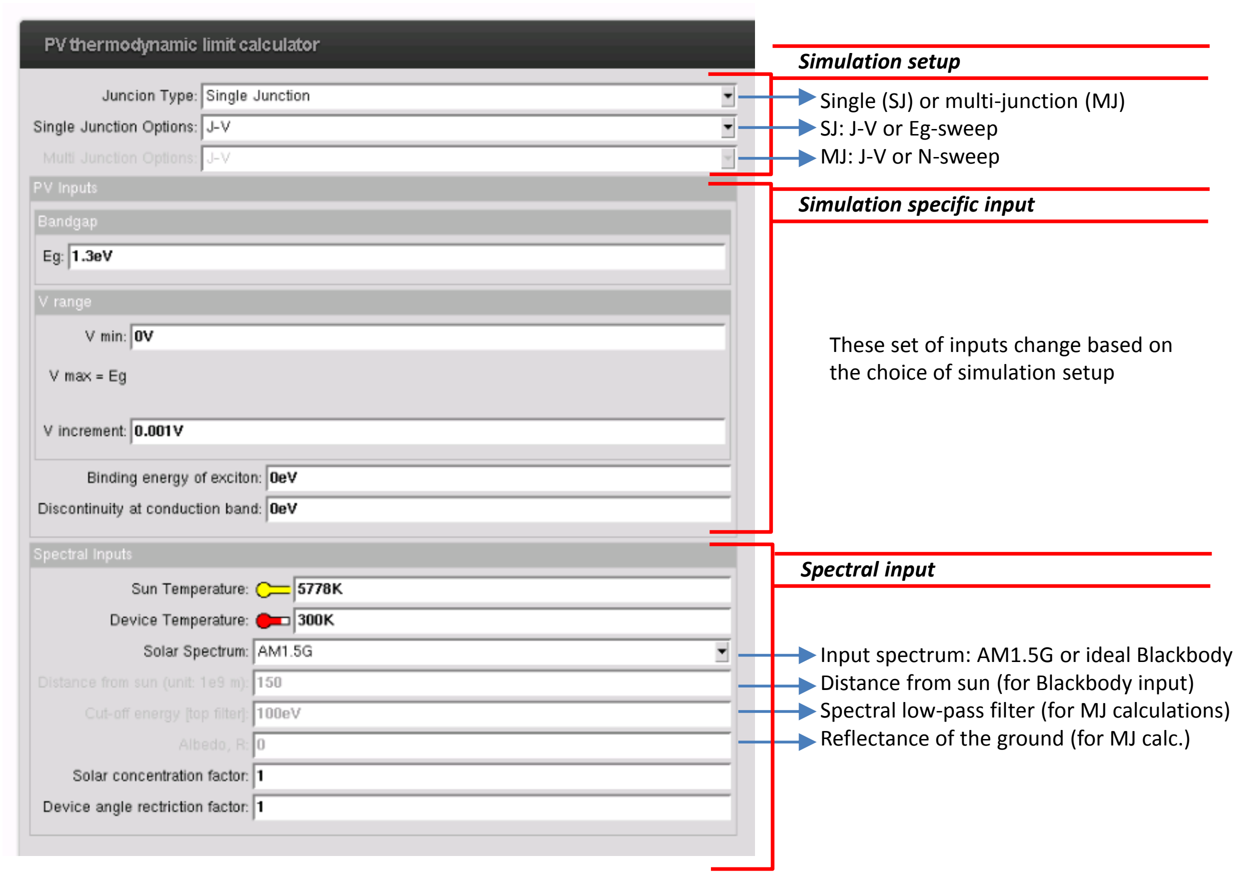
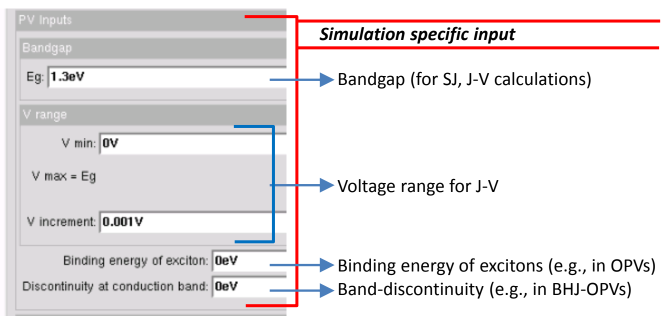


Figure 1: Simulation setup and input parameter summary for PVlimits tool.

2.1.2 PV inputs

The input parameters available in this pane depend on the choice of simulation setup.

<table>
<tr><th>Single junction (J-V)</th><th>Single junction (Eg-sweep)</th></tr>
<tr><td>


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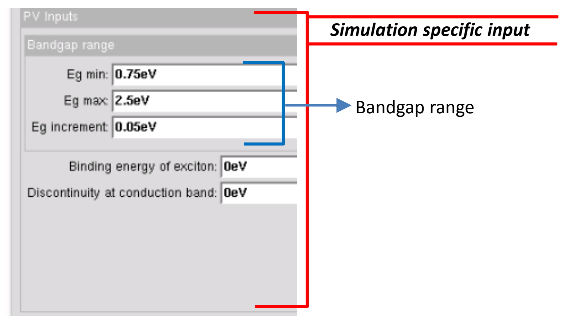

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</table>

The binding energy of exciton is relevant for an excitonic solar cell (e.g., OPVs). The band-discontinuity restricts radiative emission primarily to the heterojunction (HJ) or the cross-gap. The thermalization and the band-discontinuity are assumed to provide energy for probable exciton dissociation in the system [6]. All the calculations for the single junction PV are based on refs [2], [6].

For the multi-junction simulations, the number of subcells (N) is the only input in this section. (NOTE: MJ solar cells simulated here are always bifacial, i.e., they emit from both front and back faces.)

2.1.3 Spectral input

The spectral input pane is the same for all the simulation setups. This input-set is briefly mentioned in Fig-1. The spectral input parameters are explained in more details in the following table:

Parameter	Default value	Comments
Sun temperature	5778 K	Temperature of the source (temperature can be changed for other systems, e.g., for thermo-photovoltaics). NOTE: keep at default while using AM1.5G.
Device temperature	300 K	
Spectrum	AM1.5G	[AM1.5G or ideal Blackbody]
Distance from sun	150 (*1e9m)	This is the distance from the source to the device. The distance will change the incident solid angle.
Cut-off energy [top filter]	100 eV	This allows a low-pass energy filter at the top. In a compound system, the high energy photons can be redirected for other applications.
Albedo, R	0	Range: [0, 1]. This is the effective scattered light from the surroundings to the back of the solar module
Concentration factor	1	Range: >0. For a concentrator PV, this factor is ≥ 1. However, for a cloudy day or lower intensity input, the simulator also allows concentrator factor of $[0,1]$.
Angle restriction factor	1	The factor by which the emission solid angle is restricted.

(For some relevant distances from the sun see: http://www.pveducation.org/pvcdrom/properties-of-sunlight/solar-radiation-in-space)

2.2 Simulation Output

Once the simulation is done using a choice of input-sets, the results can be found from the drop-down list. Results can be compared for different sets of 'PV inputs' and 'Spectral inputs'. (NOTE: we recommend clearing the results before simulating a new 'Simulation setup').

The summary of the outputs are given below:

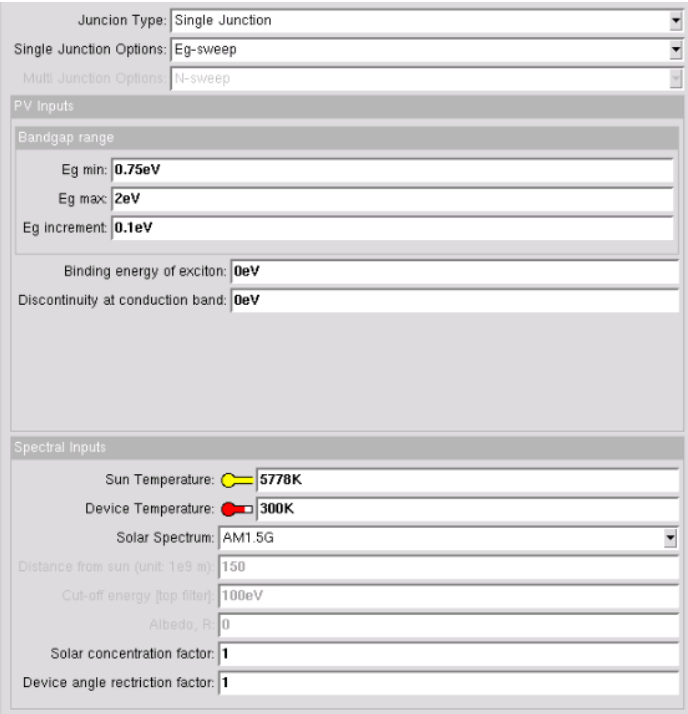
Output	Description
Single junction J-V	
Fraction of incident solar radiation	Output power and all the power loss components normalized to the net input solar power
J, Jopt vs. V	J-V curve (J in mA/cm^2)
Simulation log	List of output parameters. NOTE: net solar illumination is the incident flux (before any concentration)
Single junction Eg-sweep	
Fraction of solar radiation	Output power and all the power loss components normalized to the net input solar power. See [2], [6] for details and physics.
Efficiency matrix	This is the set of values in the plot of 'fraction of solar radiation' or power budget. The first column is the bandgap Eg (eV). The subsequent columns contains the power components mentioned in the previous plot.
Efficiency vs Eg	
Jsc vs Eg	
Voc vs Eg	
FF vs Eg	
Voc, Vopt vs Eg	
Jsc, Jopt vs Eg	

Output	Description
Multi-junction J-V	
Jsc, J_fit vs Eg	Blue line: Jsc vs Eg. Red line: a straight line fit for Jsc vs Eg for 0.5 to 1.7eV. The fitting equation: Jsc = J_SUN (1- beta*Eg). The fitting parameters are given in the simulation log
J, Jopt vs V	The J-V curve
Subcell index vs Eg	The bandgap sequence in the optimized tandem
Simulation log	Summary of output parameters
Multi-junction N-sweep	
Jsc, J_fit vs Eg	[explained as before]
Simulation log	Summary of output parameters
Eg vs no of subcells	This shows the optimized tandem bandgap-sets for N-subcells
Eg matrix	The bandgap values from the previous plot is given in this matrix
Normalized efficiency vs N	The output is normalized to 1-sun to find the normalized efficiency
Voc, Vopt vs N	
Jsc vs N	

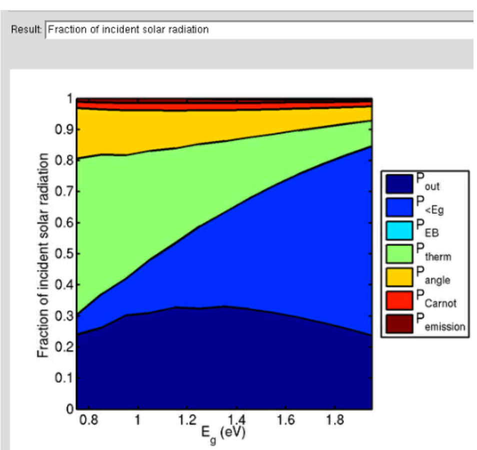
3 Illustrative Example

3.1 Single junction Eg-sweep

Input set: (Eg-sweep with AM1.5G illumination)



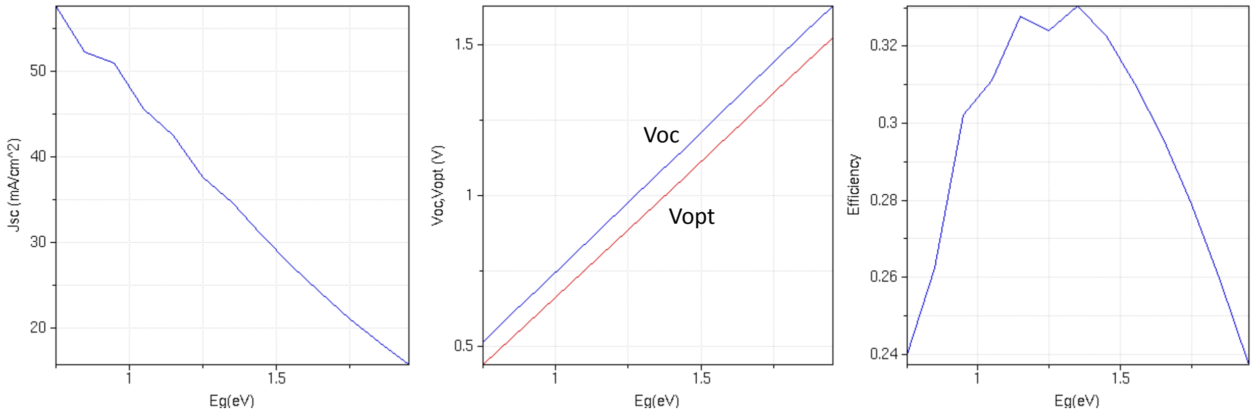
Output sets: (power budget; for physics see [2], [6])



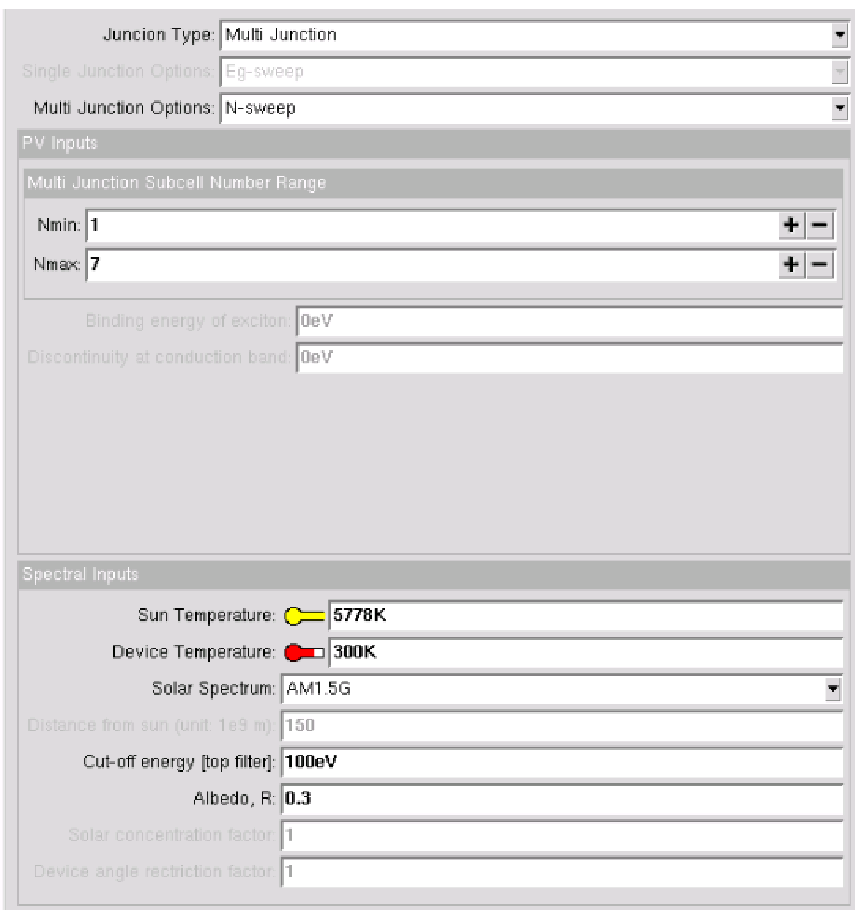
Result: Efficiency Matrix

Eg (eV)	Output, P_{out}	Below Eg, $P_{<Eg}$	Binding energy loss, P_{EB}	Thermalization loss, P_{therm}	Angle entropy, P_{angle}	Carnot loss, P_{Carnot}	Emission loss, $P_{emission}$
0.7500	0.2400	0.0636	0.0000	0.5039	0.1614	0.0212	0.0234
0.8500	0.2625	0.1069	0.0000	0.4493	0.1471	0.0219	0.0213
0.9500	0.3020	0.1182	0.0000	0.3975	0.1446	0.0241	0.0201
1.0500	0.3110	0.1714	0.0000	0.3492	0.1303	0.0240	0.0168
1.1500	0.3277	0.2066	0.0000	0.3051	0.1218	0.0246	0.0149
1.2500	0.3241	0.2644	0.0000	0.2651	0.1082	0.0237	0.0132
1.3500	0.3306	0.3026	0.0000	0.2291	0.1000	0.0237	0.0120
1.4500	0.3226	0.3553	0.0000	0.1963	0.0894	0.0227	0.0104
1.5500	0.3105	0.4084	0.0000	0.1672	0.0792	0.0215	0.0096
1.6500	0.2961	0.4599	0.0000	0.1416	0.0700	0.0203	0.0082
1.7500	0.2788	0.5106	0.0000	0.1191	0.0614	0.0189	0.0073
1.8500	0.2591	0.5603	0.0000	0.0994	0.0535	0.0174	0.0061
1.9500	0.2375	0.6093	0.0000	0.0823	0.0460	0.0158	0.0049

Output sets: (Jsc, Voc, Vopt, efficiency)

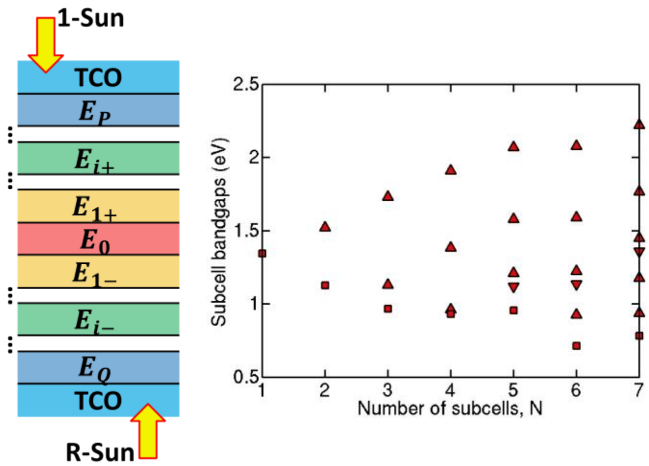


3.2 Multi-junction N-sweep: (albedo, R=0.3)



Output sets: (optimized badgaps for tandem)

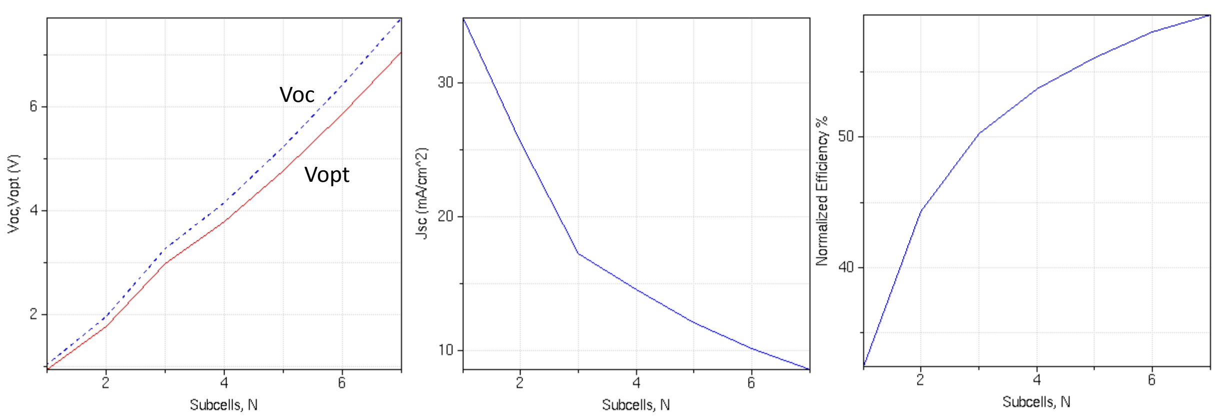
For conventional tandems, the bandgaps of the subcells always have decreasing values starting from top. However, for bifacial tandem there are sources from both sides—therefore, scanning from top to bottom subcells: top most subcell has the largest bandgap, then the bandgap reaches some minimum (E_0) and then increases again. In the output plot for bandgaps vs number of subcells: the squares (□) mark E_0. The Δ and ∇ markers represent bandgaps for the front $\{i+\}$ (subcells on top of E_0) and bottom $\{j-\}$ (subcells below E_0).



Eg matrix:

1.3442	1.5212	1.7302	1.9086	2.0685	2.0781	2.2210
NaN	1.1255	1.1296	1.3820	1.5777	1.5885	1.7667
NaN	NaN	0.9660	0.9602	1.2107	1.2229	1.4488
NaN	NaN	NaN	0.9316	0.9565	0.9260	1.1750
NaN	NaN	NaN	NaN	1.1177	0.7146	0.9370
NaN	NaN	NaN	NaN	NaN	1.1337	0.7831
NaN	NaN	NaN	NaN	NaN	NaN	1.3594

Output sets: (Jsc, Voc, Vopt, efficiency)



4 References

[1] W. Shockley and H. J. Queisser, "Detailed Balance Limit of Efficiency of p-n Junction Solar Cells," *J. Appl. Phys.*, vol. 32, no. 3, p. 510, 1961.

[2] L. C. Hirst and N. J. Ekins-Daukes, “Fundamental losses in solar cells,” *Prog. Photovolt: Res. Appl.*, vol. 19, no. 3, pp. 286–293, 2011.
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[4] M. R. Khan and M. A. Alam, “Thermodynamic limit of bifacial double-junction tandem solar cells,” *Applied Physics Letters*, vol. 107, no. 22, p. 223502, Nov. 2015.
[5] M. A. Alam and M. R. Khan, “A Markov Chain Approach for Defining the Fundamental Efficiency Limits of Classical and Bifacial Multi-junction Tandem Solar Cells,” 2016.
[6] M. R. Khan and M. . Alam, “Critical binding energy for exciton dissociation and its implications for the thermodynamic limit of organic photovoltaics,” in *Device Research Conference (DRC), 2014 72nd Annual*, 2014, pp. 281–282.