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Research article

Parameters critically affecting the open circuit voltage of an organic solar cell

Pelote Elvis Pepa [a], David Afungchui [a,c,*], Olivier Holtomo [a,b], Joseph Ebobenow [c]

[a] Department of Physics, Faculty of Science, The University of Bamenda, P. O. Box 39, Bambili, Cameroon
[b] Department of Physics, Faculty of Science, The University of Maroua, P. O. Box 814, Maroua, Cameroon
[c] Department of Physics, Faculty of Sciences, University of Buea, SWR, Cameroon

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ABSTRACT

This paper investigates the influence of different parameters on the open circuit voltage of an organic solar cell (OSC) and how the open circuit voltage impacts the cell's power conversion efficiency. These parameters include temperature, light intensity, recombination, charge carrier density, charge carrier mobility ratio, and the reverse saturation current. Organic solar cells' power conversion efficiency is still far from ideal and is currently about 20 %. In the approach, mathematical expressions governing these parameters are established and simulations are then performed in which all other parameters are held at their optimal values and one parameter of interest is varied within a predetermined range. It is shown that the open circuit voltage (V_{oc}) can theoretically reach a value of about 2.34 V if the following parameters are maintained optimal: light intensity, charge-carrier density ($1 \times 10^{18} cm^{-3}$), charge carrier mobility ratio (10) and cell temperature (320 K). It is shown that the open circuit voltage (V_{oc}) is negatively impacted by recombination (up to 30 Ω). Lastly, the power conversion efficiency is predicted to be 20 % at 0.63 V and can reach a theoretical value of 37 % at a V_{oc} of 1.0 V, at a power intensity input of 6.578 w/m^2, and a fill factor of 0.89 (max for silicon).

1. Introduction

Organic photovoltaic is a recent technology that portrays a wide range of advantages such as: having modules built with light-weight and flexible organic materials rendering them appropriate for attachment as an accessory to clothing and purses; exhibiting partial transparency; simple incorporation into additional goods; having new market prospects, such as wearable photovoltaics; much-reduced production costs when compared to traditional inorganic technologies; continuous manufacturing of OPV with cutting-edge printing equipment; minimal environmental risks and quick energy payback periods and because they are multicoloured, they may be made to match the colour of purses and clothes.

Organic solar cells have been demonstrated as the potential choice for the next generation of photovoltaic (PV) devices. From the manufacturing perspective, the device processing of an organic solar cell (OSC) is easier, compared to other recent PV technologies [1]. The high absorption coefficients demonstrated in organic semiconductors [2] allow the use of extremely thin films [3,4]. The manufacturing costs of OSCs are cheaper, and this combined with fewer materials required for their production, put OSCs in an

* Corresponding author. Department of Physics, Faculty of Science, The University of Bamenda, P. O. Box 39, Bambili, Cameroon.
E-mail addresses: peloteelvis@ahoo.com (P.E. Pepa), afungchui@yahoo.fr (D. Afungchui), holtomo@yahoo.fr (O. Holtomo), ebobenow@gmail.com (J. Ebobenow).

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advantaged position in the future PV market. Organic photovoltaic (OPV) devices are also characterised by a system of aggregate small molecules which have boosted the power conversion efficiency by up to 12 % as reported in Ref. [5]. The bulk heterojunction (BHJ) type of OPV devices, which is a blend of an electron-donor small molecule material and an electron-acceptor material is now the standard choice for applications, owing to the above advantages and presenting the best performance efficiency (PCE) [6].

Despite these advantages coupled with the flexibility of OPV cells and lower cost, a major shortcoming according to recent research on the technology remains their low power conversion efficiency.

When an OPV device is not connected to any circuit, the electrical potential difference between its two terminals is known as the open circuit voltage (V_{oc}). The highest value of V_{oc} measures the approximate energy difference between the donor's HOMO level and the acceptor's LUMO level [7]. The link between the energy levels at the donor-acceptor (D-A) interface and the open circuit voltage for various bulk heterojunction solar cells was investigated by Scharber et al. in 2016 [8]. One of the most significant fullerene derivatives, PCBM, was utilized as the acceptor material for each device, whereas different donor materials were used. This work led to the derivation of a straightforward relationship between the HOMO of the donor material and the V_{oc} of the device, expressed in Eq. (1) [9].

$$V_{OC} = \frac{1}{q}\left(\left|E_{HOMO}^{Donor}\right| - \left|E_{LUMO}^{Acceptor}\right|\right) - 0.3V \tag{1}$$

where $E = qv$ (potential difference being work done per unit charge), q is the elementary charge, E_{HOMO}^{Donor} is the energy level of the highest occupied molecular orbital of the donor material, $E_{LUMO}^{Acceptor}$ is the energy level of the Lowest unoccupied molecular orbital of the acceptor material

But rather than being theoretically derived, these results are based on practical analysis. This link is however implicitly questioned by other researchers on the genesis of V_{oc} [10], highlighting the fact that, unlike silicon p-n junction solar cells, the formation of V_{oc} in bulk heterojunction organic solar cells is still poorly understood. In effect it is pointed out in Ref. [10] that, models which perceive polymer semiconductors materials as undoped need some revision to capture the effect of band bending (depletion zones) and the injection of minority carrier and storage in the diode bulk. Currently, research effort is being done to increase the open-circuit voltage (V_{oc}), which is now slightly greater than 1 V for single junction OSC and about 2.03 V for some tandem cells [29]. It is intended in this work to contribute to this on-going effort through theoretical analyses and numerical simulations with the target to improve the open-circuit voltage (V_{oc}).

This work focuses on modelling an Organic Solar Cell (a belt equivalent circuit model). The model of the OSC taken into consideration here is derived from the Mazhari's model of the OSC [11]. In the DC analysis of the equivalent circuit model, recombination effects and charge extraction resistances are captured as diodes (that is, small voltage sources and resistors) and not just resistors. Using the model, various parameters that affect V_{oc} are studied through equations derived from the electrical circuit model. The model is formulated based on electrical circuit equations. All derived equations are substituted into the electrical equations of the OSC both in the dark condition and light conditions where simulations are done to see the trends on various parameters that affect V_{oc} of the OSC. The main limitation of the model is the generic nature that does not offer the possibility to test specific OSC materials, which take into consideration some morphological parameters. The results obtained are in agreement qualitatively in all cases with experimental predictions from literature and quantitatively in some cases. It is believed that by enhancing the properties of organic solar cells and driving the efficiency to comparable levels as that of inorganic solar cells will greatly shift technology towards the production more of OSC as they are much cheaper to produce as highlighted above.

2. Modelling of an organic solar cell

Mazhari's organic solar cell model is adopted in the foregoing analyses [11]. The organic solar cell is modelled as a circuit element operating as a light-regulated current source. In the circuit, this current source generates a given amount of direct current at a fixed light intensity that transits through a Shockley's Diode, which is connected in parallel to the current source. An OSC's ability to

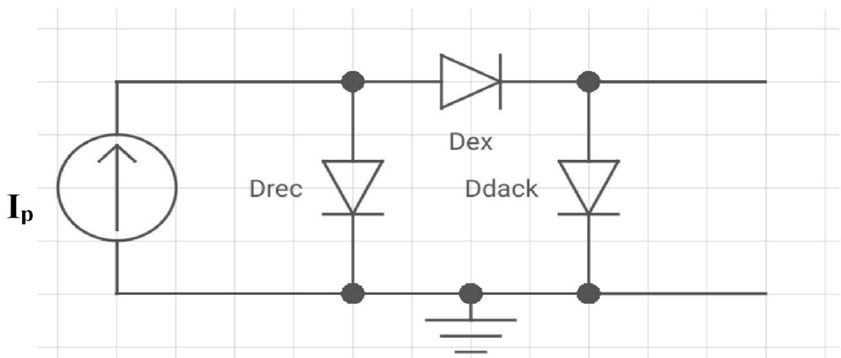

Fig. 1. Equivalent circuit model for an organic solar cell in the absence of parasitic series and shunt resistances.

generate current is impeded jointly by the phenomenon of exciton recombination and charge carrier extraction at the electrodes. In the model, these recombination effects are represented by a forward-biased diode D_{rec} (silicon diode $V_{01} = 0.7$ V and $R_{rec} = 25\ \Omega$) connected in parallel to the current source. A second diode, D_{ex} (germanium diode $V_{02} = 0.3$ V and $R_{ex} = 5\Omega$) models the impact of the resistance triggered by charge extraction at the electrodes.

In Fig. 1, D_{dack}, also known as Shockley's Diode, is regarded as a perfect diode governed by Shockley's diode equation. This diode equation is derived based partly on the presumption that the diode would not have a depletion layer or built-in potential. In the forward bias mode, an ideal diode provides resistance to the flow of current and has a built-in potential of 0.7 V for silicon-based diodes and 0.3 V for germanium-based diodes. The impact of recombination in OSCs is modelled by this resistance. The diodes' inherent potential will have an impact on the cell's open circuit voltage.

An organic solar cell generates no current when it is in the dark condition because it produces no excitons, has no recombination effects, and has no exciton dissociation. Within the cell, there is a built-in potential difference. This is a type of diode capacitor because the donor and acceptor materials have different energy potentials, which causes an internal electric field to build up between the two plates. As seen in Fig. 2, this can be represented as an Ideal Shockley's diode in an open circuit.

The current flowing through the diode I_D if the circuit is closed in the absence of the current source (short circuit current I_{sc}) is given by Ref. [12]:

$$I_D = I_O\left(e^{\frac{qV_0}{RT}} - 1\right) \tag{2}$$

where I_0 is the reverse saturation current, R is the Boltzmann's constant, q is the electronic charge, and T is the temperature. Eq. (2) indicates that the cell will behave as an intrinsic semiconductor whereby the number of holes (P_p) and electrons (P_n) increase with increasing temperature in the absence of light. Further evidence for this comes from the Boltzmann's equation [22].

$$P_p = P_n e^{\frac{V_O}{V_T}} \tag{3}$$

where P_p is the number of holes, P_n the number of electrons, V_0 the build in potential of the diode and V_T is the thermal voltage of the diode.

2.1. Relationship between temperature (T), recombination effects (R_{rec}), and open circuit voltage (V_{oc})

An OSC illuminated by light of a certain frequency and intensity will generate some direct current, which will in turn initiate some resistance and will be subjected to some recombination effects as the charge carriers reach the electrodes. As a consequence, the net short-circuit current of the OSC will drop, decreasing the solar cell's power conversion efficiency. An OSC under illumination is modelled as presented in Fig. 3.

An application of Kirchhoff's Current and voltage laws result in the open circuit voltage expressed as:

$$V_{oc} = I_p R_{rec} - I_O\left(e^{\frac{qV_0}{RT}} - 1\right)(R_{rec} + R_{ex}) + (V_{01} - V_{02}) \tag{4}$$

Eq. (4) establishes the relationship between the open circuit voltage (V_{oc}), temperature (T), and recombination effects (R_{rec}). V_{01} has a value of 0.7 V for silicon diodes and V_{02} take a value of 0.3 V for Germanium diodes. The silicon diode is preferred here to model recombination effects because it offers a higher resistance compared to other diodes. R_{ex} represents the resistance at the electrodes, I_0 is the reverse saturation current, I_p is the generated current, and V_T is the thermal voltage. V_T is expressed as:

$$V_T = \frac{RT}{q}, \tag{5}$$

and has a value of approximately 26 mV at room temperature (300 K). The rate of exciton generation is denoted as I_p and the rate of exciton recombination as R_{rec}. The highest forward-biased resistance of a silicon diode is 25 Ω, while a germanium diode may operate at a maximum temperature of 363 K and has a maximum forward-biased resistance of 5 Ω. A silicon solar cell can produce a maximum current of 46 mA/cm^2.

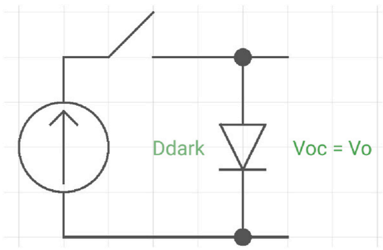

Fig. 2. The circuit diagram of the modelled organic solar cell in the dark.

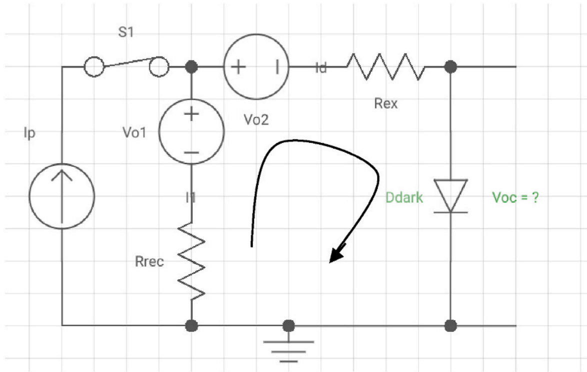

Fig. 3. Model of organic solar cell under light condition.

In what follows, the factors that influence exciton generation I_p like temperature and light intensity will be investigated.

2.2. *The impact of light intensity on the open-circuit voltage of the organic solar cell*

Light intensity is described as the number of photons in a beam, that is [13]:

$$I_L = h\nu \varnothing_{ph} \tag{6}$$

In Eq. (6), I_L denotes the light intensity, h is the Planks constant (6.62559×10^{-34}Js), and $\varnothing_{ph}$ is the photon flux. The short circuit current (I_{sc}) produced by a photovoltaic material is directly proportional to the intensity of the incident light. This is referred to as the number of suns (X), according to G. Bunea et al. [13], where 1 sun is equivalent to a standard lighting power of 1 kW/m^2. Mathematically, this implies that:

$$I_L = XI_{sc} \tag{7}$$

Combining Eq. (2) with Eq. (7) results in an ideal model of an OSC operating in the dark, which is expressed as,

$$XI_{sc} = I_o\left(e^{\frac{qV_{oc}}{RT}} - 1\right) \tag{8}$$

Eq. (12) can be rearranged to express V_{oc} as:

$$V_{oc} = \frac{RT}{q} In\left(\frac{XI_{sc} + I_O}{I_0}\right) \approx \frac{RT}{q} In\left(\frac{XI_{sc}}{I_0}\right) \quad for \quad I_{sc} \gg I_0 \tag{9}$$

In the case where $I_{sc} \gg I_0$, V_{oc}' can be expressed for convenience as:

$$V_{oc}' \approx \frac{RT}{q} In\left(\frac{XI_{sc}}{I_0}\right) = V_{oc} + \frac{RT}{q} InX \tag{10}$$

where

$$V_{oc} \approx \frac{RT}{q} In\left(\frac{I_{sc}}{I_o}\right) \tag{11}$$

In the event of exciton recombination and charge collection at the electrodes Eq. (4) now becomes

$$V_{oc} = I_p R_{rec} - I_O\left(e^{\frac{qV_0}{RT}} - 1\right)(R_{rec} + R_{ex}) + (V_1 - V_2) + \frac{RT}{q} InX \tag{12}$$

where X is the number of suns.

2.3. *The effect of charge density on V_{oc} of an organic solar cell*

In the dark condition, $V_0 = V_{oc}$ or the open circuit voltage is equal to the built-in potential of Shockley's diode V_0. The energy gap is defined as [9]

$$E_0 = -V_0 q \tag{13}$$

when the OSC is in dark conditions (Open circuit mode with zero recombination and electrode resistance effects)

$$V_0 = V_{oc} = \frac{1}{q}\left(E_{nc}^{LUMO} - E_{nc}^{HOMO}\right) \tag{14}$$

where, the value of V_{0C}, depends on the type of the Donor/Acceptor material used.

Denoting the electron concentration as n, holes concentration as p, charge carriers concentration in the conduction band as N_c, and charge carriers concentration in the valence band as N_v, then np is expressed as [23]

$$np = N_C N_V e^{\frac{-E_g}{KT}} \tag{15}$$

The law of mass action also permits the alternative expression:

$$np = n_i^2 \tag{16}$$

The HOMO-LUMO band gap energy can then be expressed as:

$$E_g = KT\ln\frac{N_C N_V}{n_i^2}, \tag{17}$$

and it follows that

$$E_0 = KT\ln\frac{N_D N_A}{n_i^2} \tag{18}$$

From Eq. (13), which represents the model OSC in the dark condition V_0 is then expressed as,

$$V_0 = \frac{KT}{q}\ln\frac{N_D N_A}{n_i^2} \tag{19}$$

hence

$$V_{0C} = \frac{KT}{q}\ln\frac{N_D N_A}{n_i^2} \tag{20}$$

where K is the Boltzmann's constant, T is the temperature, q is the electronic charge, n_i is the intrinsic charge carrier density, N_D is the donor material charge density, and N_A is the acceptor material charge density. For silicon, the maximal intrinsic carrier concentration is $n_i = 5 \times 10^{12} cm^{-3}$. V_{oc} is dependent on the log of the Donor and acceptor concentration in the organic molecule, according to Eq. (20).

2.4. Effect charge carrier mobility on the open circuit voltage

Charge carrier mobility is governed by drift and diffusion effects. The movement of charge carriers (holes or electrons) driven by concentration gradients generates a diffusion current. Hence there is a direct proportionality between the diffusion current density and the concentration gradient.

The proportionality is expressed for electrons and holes as:

$$J_n \propto \frac{dn}{dx} \tag{21}$$

and

$$J_P \propto \frac{dp}{dx} \tag{22}$$

Where J_n and J_p are the diffusion current densities generated by electrons and holes respectively.

They can be further expressed as:

$$J_n = +eD_n\frac{dn}{dx} \tag{23}$$

and

$$J_p = -eD_p\frac{dp}{dx} \tag{24}$$

where D_n and D_p denote the diffusion current coefficients of the electrons and holes respectively. Taking into consideration the drift velocity, the total current densities due to the electrons and the holes are expressed respectively as [14]:

$$J_n = en\mu_n E + eD_n \frac{dn}{dx} \tag{25}$$

and

$$J_p = ep\mu_p E - eD_p \frac{dp}{dx} \tag{26}$$

These can be combined into a single expression as:

$$J = J_n + J_p \tag{27}$$

or,

$$J = \left(en\mu_n + ep\mu_p\right)E + eD_n \frac{dn}{dx} - eD_p \frac{dp}{dx} \tag{28}$$

where μ_n *and* μ_p are the electrons and holes mobility respectively and n and p are respectively the electron and hole concentration.

Unlike the diffusion current which is driven by the concentration gradients of the holes and the electrons, the drift current is caused by an internal field at the donor-acceptor interface, acting on the excitons. The energy associated with this field is expressed as [15]:

$$qV_{oc} = E_0 = 1/2\left(E_{pi} - E_{pf}\right) = -1/2\left(E_{nf} - E_{ni}\right) \tag{29}$$

where E_{pi} is the intrinsic energy level of p-type material (acceptor material), E_{pf} is the Fermi energy level of p-type material, E_{nf} is the Fermi energy level of n-type material and E_{ni} is the intrinsic energy level of n-type material. The Fermi energy level **(E_f)**, is that energy level that has 50 % probability of occupation by an electron at any temperature. The intrinsic energy level **(E_i)** is the average internal energy of the n-type or p-type material.

From semiconductor theory, the concentrations of majority charge carriers; n and p in the N-type and P-type materials are respectively expressed as [23]:

$$n = N_c \exp(-E_0 / 2K_B T) \tag{30}$$

and

$$p = N_v \exp(E_0 / 2K_B T) \tag{31}$$

Putting these various contributions into Eq. 28 give:

$$J = \left(e\mu_n N_c \exp(-2E_0 / K_B T) + e\mu_p N_v \exp(E_0 / 2K_B T)\right)E + eD_n \frac{dn}{dx} - eD_p \frac{dp}{dx}. \tag{32}$$

or,

Considering the model of our OSC in the dark condition, from equation (29)

$$qV_{oc} = E_0\ J(V_{oc}) = \left(e\mu_n N_c \exp(-qV_{oc} / 2K_B T) + e\mu_p N_v \exp(qV_{oc} / 2K_B T)\right)E + eD_n \frac{dn}{dx} - eD_p \frac{dp}{dx} \tag{33}$$

However, the current does not flow under open circuit conditions, expressed as:

$$d\left(\frac{J(V_{oc})}{d(V_{oc})}\right) = 0, \tag{34}$$

or,

$$\frac{eq\mu_n N_c}{K_B T} \exp(-qV_{oc} / 2K_B T) = \frac{qe\mu_p N_v}{K_B T} \exp(qV_{oc} / 2K_B T), \tag{35}$$

Choosing an optimum operating condition characterised in this situation by, $N_c = N_v$, leads to:

$$V_{oc} = \frac{K_B T}{q} \ln\left(\frac{\mu_n}{\mu_p}\right), \tag{36}$$

from which it can be concluded that the charge carriers mobility ratio is a multivariable function of temperature, electric field strength, electrons and holes concentrations, and impurities which increase resistance.

2.5. The impact of exciton recombination on V_{oc}

Exciton current Ip is lowered by recombination effects. A rising R_{rec} in an organic solar cell system will provoke a decrease in I_p which is accompanied by a linear decrease in V_{oc}. The variation of V_{oc} against I_p is obtained by rearranging Eq. (12) as expressed in Eqs.

(37) and (38). A feasible and reasonable range of I_p is obtainable from Eq. (38) by substituting the lowest and highest values of the recombination factor R_{rec}, while all other parameters are maintained at their optimal values.

$$V_{oc} = \left(I_p - I_O\left(e^{\frac{qV_0}{RT}} - 1\right)\right)R_{rec} - I_O\left(e^{\frac{qV_0}{RT}} - 1\right)(R_{ex}) + (V_1 - V_2), \tag{37}$$

from which,

$$I_p = \frac{V_{oc} + I_O\left(e^{\frac{qV_0}{RT}} - 1\right)(R_{ex}) - (V_1 - V_2)}{R_{rec}} + I_O\left(e^{\frac{qV_0}{RT}} - 1\right) \tag{38}$$

Eqs. (37) and (38) demonstrate that exciton recombination is a parameter that will impact the value of V_{oc} in an organic solar cell. The Recombination parameter is very important in the cell because it prevents an imminent disintegration of the organic material by avoiding an uncontrollable increase of the majority charge carriers.

2.6. Effects of the reverse saturation current on V_{oc}

The reverse saturation current is made up of a portion of the reverse current in a semi-conductor diode resulting from the minority charge carriers that diffuse from the neutral to the depletion areas. This diffusion process goes on until the depletion layer is built up preventing further diffusion. At this stage, an internal electric field is set up causing hole diffusion from the p-type region to the N-type region and electron diffusion in the reverse direction.

When the OSC is illuminated or subjected to some finite temperature, the bonds will break causing a rise in the reverse saturation current.

In the dark state, the organic solar cell is modelled as a Shockley's diode given by Eq. (2); from which V_{oc} is expressed as:

$$V_{oc} = \frac{RT}{q} In\left(\frac{I_D + I_0}{I_0}\right) \tag{39}$$

Knowing that $I_D \gg I_0$, this expression simplifies to:

$$V_{oc} = \frac{RT}{q} In\left(\frac{I_D}{I_0}\right) \tag{40}$$

This equation gives the relationship between the open circuit voltage and reverse saturation current I_0. For a given I_p, representing the current source value, and from the current divider rule, I_D is expressed from Fig. 3 as:

$$I_D = \left(\frac{R_{rec}}{R_{ex} + R_{rec}}\right) I_p \tag{41}$$

Where I_D is the current through the Shockley's diode

3. The effect of open circuit voltage on the power conversion efficiency (PCE) of an organic solar cell

An organic solar cell's power conversion efficiency (PCE) is expressed as a function of the fill factor (FF), the short circuit current, the open circuit voltage, and the incident light intensity. The fill factor (FF) here is a measure of the maximum electric power production per unit active area of the OSC. Eqn. (38) is used to calculate PCE as follows [16].

$$FF = \frac{(JV)_{max}}{J_{sc} V_{oc}}, \tag{42}$$

$$PCE = \frac{V_{OC}\, J_{SC}\, FF}{P_{in}} \times 100\% \tag{43}$$

where FF is the fill factor, J_{sc} is the short circuit current and P_{in} is the intensity of incident light. Silicon solar cells present a maximum short circuit current of 0.042 A/cm^2. The maximum fill factor for a silicon solar cell is approaching 0.89. The average intensity of one sun on Earth's surface is 1000 W/m^2.

4. Simulation results and discussions

Simulations are done in this section where all other parameters are maintained at their optimal values while one parameter is changed within a specified range.

4.1. Variation of V_{oc} with temperature

Eq. (4) is used in Fig. 4 to display the trend of V_{oc} with temperature. The recombination parameter is represented by a silicon-based diode with a built-in voltage (V_{01}) of 0.7 V and resistance of 25 Ω in this equation, while the extraction resistance at the electrodes is represented by a germanium diode with a built-in voltage (V_{02}) of 0.3 V and an internal resistance of 5 Ω. At an I_p value of 0.02 A, the current source is retained. The temperature fluctuates between 200 K and 340 K. We see that the open circuit voltage of the simulated organic solar cell decreases from a maximum value of 0.74 V when the temperature is 200 K.

Eq. (1)'s representation of the open circuit voltage serves as the foundation for an explanation of Fig. 4. The open circuit voltage of organic solar cells is a measure of the widening of the band gap between the LUMO and HOMO at low temperatures [9,17]. When comparing these findings to experimental studies, it can be seen that (Brus et al., 2021) observed a similar tendency where V_{oc} drops with temperature, in their study on Temperature and Light Modulated Open-Circuit Voltage in Nonfullerene Organic Solar Cells [25]. The same trend was also experience by (tang et al. 2020) showing a decrease in V_{oc} from low temperatures to increasing temperatures [26]. Thus the relationship of temperature with the open circuit voltage can be pursued so that cell performance may be optimized when used in realistic applications. Ideally, the target is to engineer OSC's to work under standard conditions. Except for low temperature application, attempts to incorporate cooling mechanisms to enhance V_{oc} in OSC's is a possibility but will however add to the complexity and the cost of system.

4.2. The relationship between V_{oc} and light intensity (number of suns) in an OSC

Eq. (12) can be used to increase the number of suns, which will consistently raise V_{oc}, to higher values at different temperature, as shown in Fig. 5.

Exciton concentration rises with light intensity (more charge carriers are photo-generated in the active layer with an increase in the number of suns), which explains the result seen in Fig. 5. This pattern is consistent with the findings of Naveen Kumar et al. (2015) [18]. According to their review, for polymer: fullerene BHJ solar cells, the open-circuit voltage varies logarithmically with illumination intensity (Voc vs ln(I)). This demonstrated a linear rise in Voc with light intensity. The trend is validated by the experimental works carried out by (Ryu et al., 2021, Benesperi et al. 2022) who experimentally recorded an increase in Voc with an increase in the percentage of light intensity [30,31].

4.3. The relationship between current generated by the cell (I_p) and recombination

The dependency of I_p with recombination effects R_{rec} is depicted in Fig. 6. Eq. (38) is used in the simulation to get this outcome. The current generated by the cell decreases from an optimal value of 1.5 A to vanishingly small values when the recombination increases from near zero to 25 Ω, which is the actual resistance of a silicon diode, and when all other parameters are kept at optimal values (i.e., $V_0 = 0.3$ V, $q = -1.6 \times 10\text{-}19$ C, T = 330 K, $R = 1.38 \times 10^{-23}$ J/K, $R_{ex} = 5$ Ω, $V_1 = 0.3$ V, $V_2 = 0.7$ V, $I_0 = 1.82 \times 10^{-11}$ A, and $V_{OC} = 1$ V).

The explanation for the results shown in Fig. 6 is that an organic solar cell can only produce a significant amount of current when a significant quantity of exciton dissociation occurs at the donor-acceptor interface of the cell. The free charge carriers that make up the cell's current won't be produced if dissociation doesn't happen. The distance between the exciton and the D/A interface (which may be adjusted by selecting the cell's morphology), the diffusion rate of the exciton, the concentration of charge carriers, and the exciton lifetime all impede this separation. An organic solar cell will provide a higher current if recombination is kept to a minimum. This outcome is consistent with research conducted by Frédéric Laqua et al. (2017), who found that exciton recombination is the primary cause of power losses in organic solar cells [19]. These results are validated by experimental results obtain by (Liu and Li, 2011) who revealed that monomolecular recombination is the primary loss mechanism in OSCs [32].

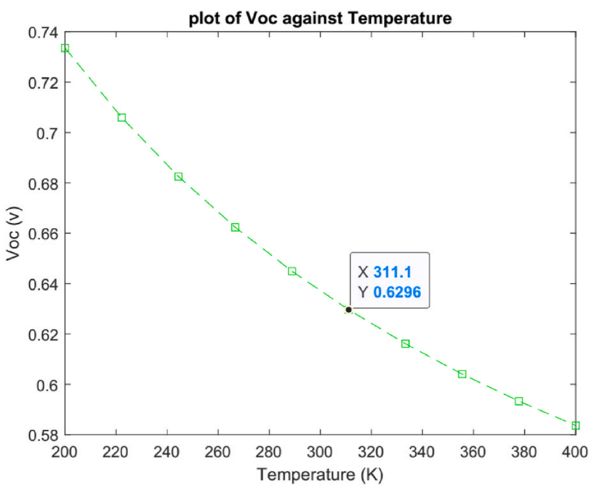

Fig. 4. Variation of V_{oc} with temperature.

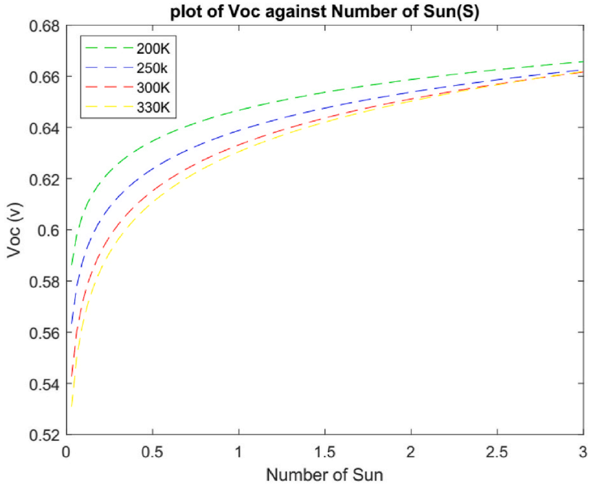

Fig. 5. The variation of V_{oc} with light intensity.

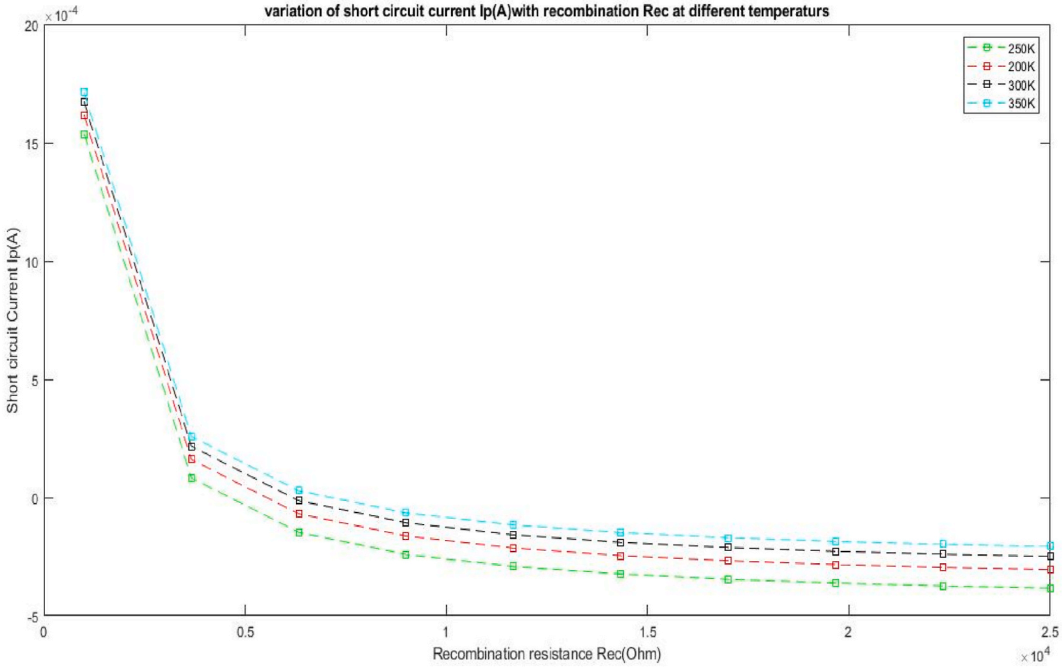

Fig. 6. The variation of cell current generated (short circuit current) (I_p) with recombination R_{rec} (Ω).

4.4. The relationship between V_{oc} and input current of organic solar cell (Ip)

The result in Fig. 7 shows the influence of I_p on the open circuit voltage V_{oc}. This result was obtained using Eq. (37). With every other parameter kept constant (i.e $V_0 = 0.3$ V, $q = -1.6 \times 10^{-19}$ C, $T = 330$ K, $R = 1.38 \times 10^{-23}$ J/K, $R_{ex} = 5$ Ω, $V_1 = 0.3$ V, $V_2 = 0.7$ V, $I_0 = 1.82 \times 10^{-11}$ A) and I_p varied from 0.4 A to 1.4 A, V_{oc} increases linearly from zero to 1 V.

The idea that the concentration of free charges placed at the electrode which is comparable to the charges placed on a capacitor's plates and determines the current it will drive through helps to explain the results in Fig. 7. It also determines the strength of the current that can be pushed through. The findings of Pankaj Kumar et al. (2009) [20] with their studies utilizing an indium tin oxide (ITO)/copper phthalocyanine (CuPc) (20 nm), C60 (40 nm), bathophenanthroline (BPhen) (8 nm), and Al (150 nm) OPV device are comparable to this one. According to their findings, I_p increases linearly with illumination intensity, which is related to V_{oc}'s increase with light intensity. Pankaj Kumar et al. (2009) [20] further report that V_{oc} is nearly saturated at high light intensities, also corroborate this result as well. This result is also validated by the experimental work carried out by (Parhi et al., 2021) on organic solar cells. They

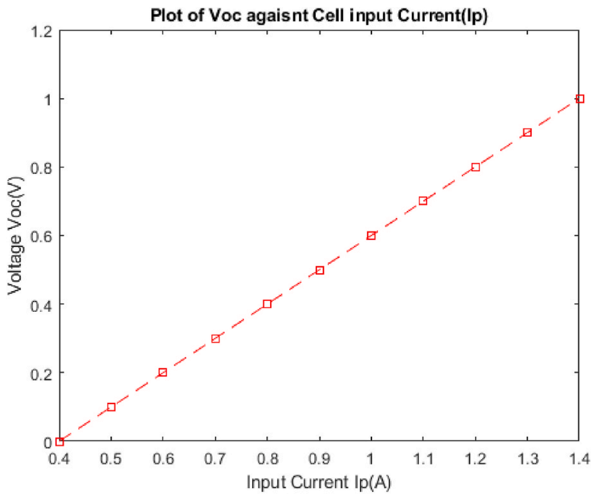

Fig. 7. The variation of V_{oc} with input current.

found that, V_{oc} increases, exhibiting a higher slope at lower intensities (less than 20 mW/cm^2) and lower slope at higher intensities from 20 mW/cm^2 to 100 mW/cm^2 [33]. In conclusion, the targeted goal of this paper has been accomplished in this instance since V_{oc} rises in response to light intensity, and light intensity and input current are directly correlated.

4.5. The relationship between the donor/acceptor concentration and V_{oc}

From Fig. 8 we see that for a given material with intrinsic carrier concentration n_i of amount $9.65x10^9 cm^{-3}$ at a temperature of 300 K, an increase in the concentration of donor and acceptor material from 0 to 1 × 10^{17} cm^{-3} at a temperature of 300 K will lead to a sharp increase in the value of V_{oc}, then approaching a saturation point where V_{oc} increases at a lower rate.

The quality of an organic material's conductivity makes it favourable to be used to build a solar cell, this explains the results in Fig. 8. Stated otherwise, a higher amount of charge carrier injection into the active layer will result in a higher V_{oc}. This pattern is consistent with the findings of Kyohei Nakano et al. [24] from 2019, who reported a linear rise in V_{oc} with carrier concentration; however, they did not address the point of saturation, which is the case in this instance. It is also critical to remember that, recombination rises linearly with donor acceptor concentration. This is a constraint on an extraordinarily high V_{oc}.

4.6. The relation between V_{oc} and reverse saturation current?

Fig. 9 shows the results obtained for a constant I_D (1 × 10^5 mA) through Shockley's diode in our model at a constant temperature of 300 K. It is observed that V_{oc} decreases from 0.25 V to 0 V) for a variation of I_0 from 0 to 1 × 10^5 mA.

Fig. 9 findings can be explained by the fact that minority charge carriers diffuse, causing reverse saturation current to flow. As more bonds in the organic molecule are broken at the Donor-Acceptor/Interface in the organic cell, the built-in potential generates an electric field that functions as an energy barrier to the flow of minority charge carriers, increasing the flow of reverser saturation current. This finding is consistent with the finding by Sean Sehyun et al. (2008) [21], who showed that reverse saturation current

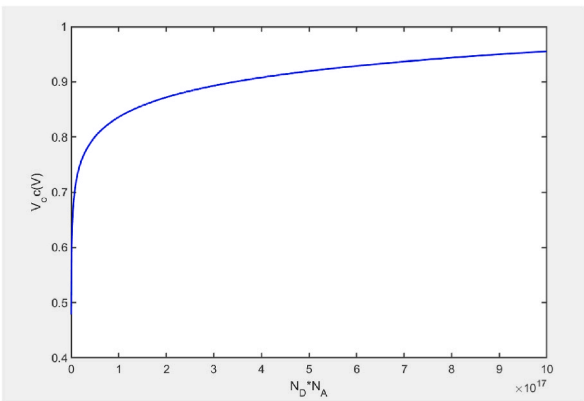

Fig. 8. Variation of V_{oc} with donor, acceptor material concentration.

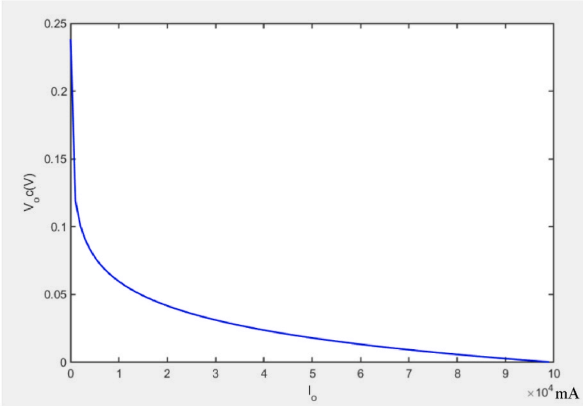

Fig. 9. Variation of Voc with reverse saturation current.

density causes V_{oc} to decrease.

4.7. The relationship between charge carrier mobility ratio with open circuit voltage

Fig. 10 shows the variation of charge carrier mobility ratio in the modelled organic solar cell with V_{oc}. This analysis is done bearing in mind that the charge carrier mobility ratio of silicon diode ranges from 0.22 to 5.55 and the mobility of electrons is 1400 cm^2/Vs and that of holes is 450 cm^2/Vs.

Since low charge mobility indicates high cell resistance and high charge mobility indicates low cell resistance, the curve in Fig. 10 makes sense. The recombination rate is high at high cell resistance, which lowers V_{oc}. Similar results are recoded by Ompong et al. [14]. When the electron mobility is greater than the hole mobility, Voc increases if the ratio $\mu_n/\mu_p > 1$. When the mobility of electrons and holes in a material are identical, the transport term's contribution to the Voc disappears. Recombination and charge carrier mobility factors as observed in the forgoing analysis can play a major role for the scalability of organic solar cell technology. In effect, recombination of charge carriers reduce efficiency since the charge carriers will not be picked up at electrodes to contribute in power production. Once the optimal values of recombination and charge carrier mobility factors are achieved for a single OSC, scalability will be done as it is the case with inorganic solar cells by arranging the cells in series or in parallel depending on the overall V_{oc} or I_{sc} that is desired.

4.8. Open circuit voltage variation with a power conversion efficiency of an organic solar cell?

Fig. 11 illustrates how an organic solar cell's power conversion efficiency is reliant on the open circuit voltage. Eq. (38) is used to get this numerical result, and the range of values for V_{oc} is [0 V–1 V]. This range of V_{oc} is the outcome of simulating an organic solar cell according model's Eq. (4).

Fig. 11 shows that from the equivalent circuit model of the OSC, we record a theoretical value of PCE of 20 % at temperatures closer to 330 K, and when V_{oc} is 0.63 V (see Fig. 4). The increase in PCE with Voc is the trend observed in OSC technology, (Zhou M et al.), in 2023 recorded PCE of 19.10 % of an OSC [27]. This trend of increase in PCE of OSC with Voc is confirmed with the experimental work

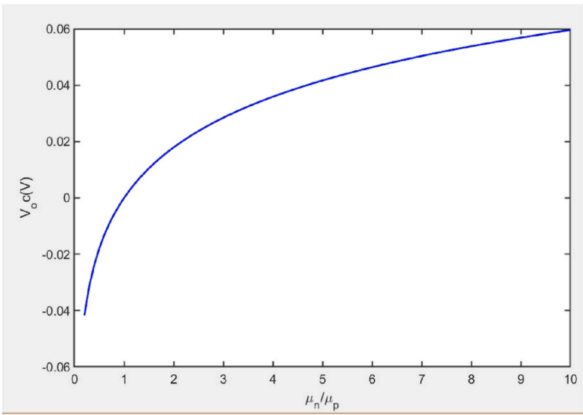

Fig. 10. Variation of V_{oc} with charge carrier mobility ratio.

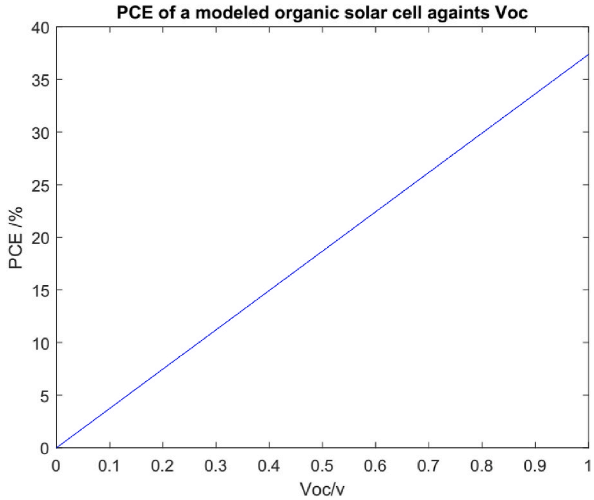

Fig. 11. Variation of PCE with V_{oc}.

Table 1
Some typical data on PCE for different V_{oc} based on single junction OSC.

SN	Voc/V	PCE/%	Year/Reference
1.	0.904	13.60	2019 [34]
2.	0.850	16.34	2020 [28]
3.	0.922	18.70	2022 [35]
4.	0.880	19.10	2023 [29]
5.	1.002 V	19.20	2024 [36]

carried out by Kang et al., in 2020 who obtained an increased in PCE from 15.7 % to 16.3 % [28]. Wang et al., in 2023 with a Voc of 1.09 for single junction OSC and 2.03 V for tandem cells experimentally recorded a certified PCE of 19.1 % and 20.3 % respectively of the constructed single and tandem OSCs [29]. Table 1 presents some optimal data of the maximum PCE for different V_{oc}.

From Table 1 we see that theoretical predictions of the current paper giving a PCE of 20.23 % for a corresponding V_{oc} of 0.63 is within range and can give more hope for the enhancement of the PCE of organic solar cells. Organic solar cells with optimum open circuit voltage will have their efficiencies enhanced. The build in voltage in the diodes that modelled recombination and charge extraction resistance at the electrode were considered in Mazhari's model of organics solar cell.

5. Conclusion

The Open circuit voltage of an organic solar cell (a model considered in this work) cell actually depends on: Temperature, Number of suns (illumination intensity), Charge carrier mobility ratio and Donor & Acceptor Concentration. When temperature increase from 200 K to 320 K, Voc drops from 0.74v to 0.63 V. Increase in the number of suns from 0 to the solar constant (~1.3suns) will lead to increase in Voc to 0.63 V, this value drops when temperature increase from 200 K to 330 K. Voc increases with increases in the charge carrier mobility ratio of electrons to holes. A Voc of nearly 1 V will be produced by donor and acceptor concentrations of the order of 1×10^{18} cm^{-3}. In addition, a rise in recombination effects within the temperature (273 K–330 K) will cause the short circuit current to drop from 1.5 A to almost zero, which will lower the voltage from 1 V to 0 V. Finally, the PCE is observed to rise from 0 to a theoretical value of 20 % as V_{oc} increases from 0 to 0.63 V. Hence PCE of an OSC is directly proportional to Open circuit voltage.

CRediT authorship contribution statement

Pelote Elvis Pepa: Writing – original draft, Software, Methodology, Investigation, Formal analysis. **David Afungchui:** Writing – review & editing, Validation, Supervision, Project administration, Methodology, Investigation, Conceptualization. **Olivier Holtomo:** Validation, Supervision, Project administration. **Joseph Ebobenow:** Validation, Supervision, Conceptualization.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Nomenclature

CT	Charge transfer
FF	Fill factor
h	Plank's constant ($m^2 kg/s$)
J	current density (A/cm^2)
OPVC	Organic photo voltaic cells
OSC	Organic Solar Cells
PCE	Power conversion efficiency (%)
q	Elementary charge (C)
R	Boltzmann's constant (J/K)
SC	solar cell
ν	Frequency of incident light (Hz)
I_L	Light intensity (cd)
D_{dack}	Shockley's Diode in the dark
D_{ex}	Diode modeling extraction resistance (Ω)
D_n	diffusion current coefficients of the electrons (cm^2/s)
D_p	diffusion current coefficients of holes (cm^2/s)
D_{rec}	Diode modeling recombination effects (Ω)
I_D	Current through the Shockley's diode (A)
I_o	Reverse saturation current (A)
J_o	Reverse saturation current density (A)
J_{sc}	Sort circuit current density (A)
P_{in}	Power of incident light (W)
P_n	Electron concentration ($electrons/cm^3$)
P_p	Holes concentration ($holes/cm^3$)
R_{ex}	Build-in-resistance of germanium diode (Ω)
R_{rec}	Build-in-resistance of silicon diode (Ω)
V_{01}	Build-in-voltage of silicon diode (V)
V_{02}	Build-in-voltage of germanium diode (V)
V_o	The build in voltage of a diode (V)
Voc	Open circuit Voltage (V)
V_T	Thermal Voltage (V/K)
E_{HOMO}^{Donor}	Homo energy of Donor material (eV)
$E_{LUMO}^{Acceptor}$	Lumo energy of acceptor material (eV)
$\varnothing_{ph}$	Photon flux. ($/sm^2$)
μ_n	Electron mobility (cm^2/Vs)
μ_p	Hole mobility (cm^2/Vs)

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