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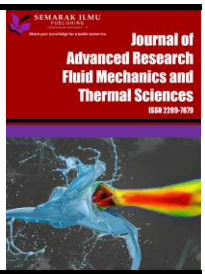


# Characterization of Chlorophyll Based Dye-Sensitized Solar Cell using General-Purpose Photovoltaic Device Model

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**ABSTRACT**

In dye-sensitized solar cells (DSSCs), light is absorbed by the sensitized dye. When light strikes the dye molecule, it absorbs photons and becomes excited to a higher energy state. This excited state allows the dye molecule to inject an electron into the conduction band of the semiconductor, generating an electric current. The selection of dye properties is very significant, as it can help to improve the performance of DSSCs. However, achieving an identical output current-voltage characteristic from the same batch of plants or fruits used as dyes is very difficult. Furthermore, improving the electrical performance, such as short-circuit current density and efficiency, of fabricated dye-sensitized solar cells is critical, as many experimental factors need to be considered. Therefore, to minimize the extra use of material resources due to the risk of unsuccessful fabrications and to obtain better performance ideally, conducting simulation-based studies is important to optimize the performance of DSSCs. The free software General-Purpose Photovoltaic Device Model (GPVDM) is a promising and interesting tool due to its free license and easy accessibility through a graphical interface for simulating optoelectronic devices, including OLEDs, OFETs, and various types of solar cells. This paper considers GPVDM, a 3-D photovoltaic device model, to simulate the proposed structure with different samples of chlorophyll dye for DSSC performance. The paper aims to characterize the high current density-voltage (J-V) of chlorophyll-based DSSCs and identify suitable photovoltaic simulation software for running simulations of chlorophyll-based DSSCs. Finally, the outcomes are compared with experimental data reported in various literature sources. The results show an enhanced short-circuit current density (Jsc) of 0.3556 mA cm$^{-2}$ for Cordyline fruticose leaves (Chl E), which is the highest among the other dyes tested. The value of simulated short-circuit current density (Jsc) is slightly different from the experimented result Jsc reported in the published paper. In conclusion, GPVDM can be considered suitable for modeling DSSCs.

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## 1. Introduction

Electricity generation consumption is expected to increase each year, which will enhance demand for fossil fuels including coal, petroleum and natural gas from the previous studies [1]. Unfortunately, [2] have reported that these vital raw materials cannot regenerate at a pace equivalent to their utilization due to the lengthy timescales—often spanning thousands of years—required for their formation. Amidst the concerns surrounding the sustainability of renewable energy resources, the solar cell, commonly referred to as the photovoltaic cell, emerges as a promising solution for meeting the escalating energy needs of the 21st century from the previous studies [3]. According to Nair *et al.*, [4], have reported that this renewable energy source harnesses sunlight to generate electricity, offering an environmentally friendly alternative to finite fossil fuels.

Organic solar cell (OSCs) represent a new generation of solar energy technologies such as dye sensitized solar cell were introduced by the previous studies [5,6]. In 1991, Professor Michael Gratzel invented the dye sensitized solar cells (DSSCs) which is this device has gained more attention for their application as their cost-effectiveness and straightforward production processes from the previous studies [7] . In dye sensitized solar cells, the function of light absorption, electron transport and hole transport are separated into different material [8]. Light is absorbed by the sensitized dye, electron transport take place in a porous semiconductor such as titanium dioxide, zinc oxide, etc., while hole transport occurs in a liquid electrolyte and charge separation takes place at the interface between photon induced electron and the dye moving into the conduction band of the solid were explained by the previous studies [9,10]. In real fabrication of DSSC, it is very difficult to have an identical output current-voltage characteristic though the same badge of plants or fruits as dyes are used. Different types pf chlorophyll dye has their own parameter where it produces different output of current density-voltage (J-V). Furthermore, improving electrical performance such as short circuit current density, efficiency, etc. of fabricated dye sensitized solar cell is very critical since lots of experimentation factors need to be considered. However, in order to minimize the extra use of material resources due to the risk of unavoidable unsuccessful fabrications and to obtain better performance ideally, the necessity of performing a simulation-based study is important to drive the performance of DSSCs.

The free software called General-Purpose Photovoltaic Device Model (GPVDM) is a free 3-D tool software which is one of the promising and interesting software due to its free license and easily accessible through graphical interface for the simulation of optoelectronic devices, including OLEDs, OFETs, and several other forms of solar cells like OSC, perovskite solar cells, CIGS and CdTe, etc was introduced by the previous studies [11]. Generally, the model can be applied the both electro and hole-drift-diffusion, and carrier continuity equation in position space, to trace the apparent movement of charges within the device. Note that several parameters play an important role in optimizing device performance [12].

In this research paper, Dye-Sensitized Solar Cells (DSSCs) are classified as third-generation solar cells, not based on their development date, but rather on the material configuration using GPVDM software. The paper primarily focuses on the effect of variation parameter in chlorophyll-based active layers toward DSSC performance. Additionally, the paper aims to characterize the high current density-voltage (J-V) of chlorophyll-based DSSC and identify suitable photovoltaic simulation software for running simulations of chlorophyll-based DSSCs. Finally, the outcomes are compared with experimental data reported in various literature sources.

## 2. Methodology
### *2.1 Device Flow*

In this section, the flow for conducting the simulation in the GPVDM software will be described in Figure 1. The flowchart illustrates two stages of the DSSC simulation process flow. First step of the simulation is to deal with the most crucial part which is device structure and parameter setting of DSSC based on semiconductor/dye/electrolyte/counter electrode such as photoelectrode type, thickness and properties (e.g. $TiO_2$, ZnO), dye and its absorption properties (e.g. chlorophyll) and electrolyte properties (e.g. potassium iodide, triiodide). All the parameters were carefully picked from practical and theoretical references. Last stages are the performance of electrical characteristics such as short circuit current density (Jsc), open circuit voltage (Voc) and the current density-voltage (J-V) curve is investigated through the GPVDM simulation software.

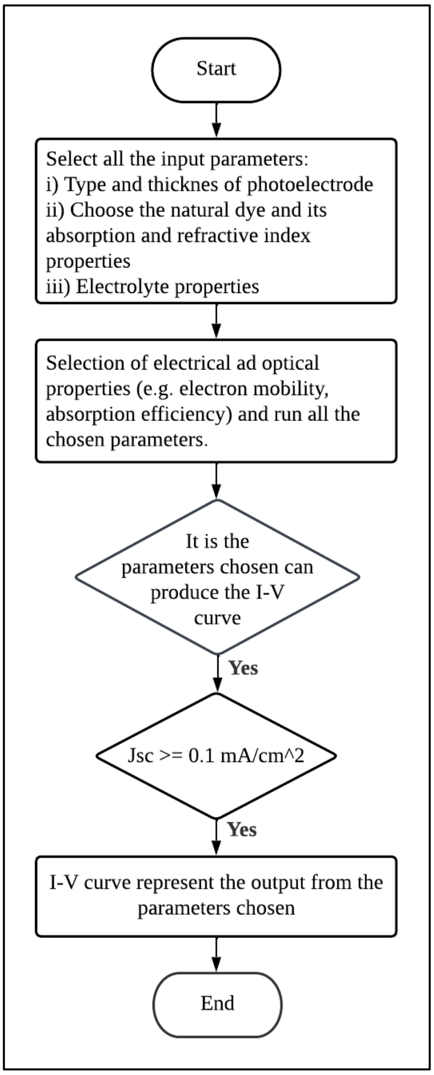


**Fig. 1.** Flowchart of simulation DSSCs

### *2.2 Device Modeling*

General-Purpose Photovoltaic Device Model (GPVDM) is a software that is found from open sources for the modelling of various type of PV cells [13]. By computing the electrical field and integrating the absorbed photon distribution throughout the solar spectrum, the transfer matrix approach is utilized to calculate the exciton production rate *G(x)* inside the active layer. The refractive index *n(λ)* and the extinction coefficient *k(λ)* indicate the optical qualities of each layer. The refractive index is used to calculate the amount of reflected and transmitted light at each interface between two adjacent layers, whereas the extinction coefficient represents a layer's capacity to absorb photons. The following equations indicate the rate of exciton formation

$$Q(x,\lambda) = \frac{1}{2} c\epsilon_0 an|E(x)|^2 \tag{1}$$

$$Q(x,\lambda) = \frac{\lambda Q(z,\lambda)}{hc} \tag{2}$$

$$G(\lambda) = \int_{Solar\ Spectrum} G(x,\lambda) d\lambda \tag{3}$$

where c is the speed of light, $\alpha = (4\pi k) / \lambda$ is the absorption coefficient, Q is the energy flow dissipation, E is the electrical field at point x within the material, and h is the plank’s constant. For electron and hole currents given by Eq. (1) to Eq. (8), the programme employs Poisson's equation Eq. (4), the carrier continuity Eq. (5, 6), and bipolar drift-diffusion Eq. (7, 8) in 1D and time domain as

$$\frac{d}{dx}\epsilon_0\epsilon_r\frac{d\emptyset}{dx} = q(n-p) \tag{4}$$

$$\frac{dJ_n}{dx} = q(R_n - G + \frac{\partial n}{\partial t}) \tag{5}$$

$$\frac{dJ_p}{dx} = -q(R_p - G + \frac{\partial p}{\partial t}) \tag{6}$$

$$J_n = q\mu_n\frac{\partial E_c}{\partial x} + qD_n\frac{\partial n}{\partial x}) \tag{7}$$

$$J_p = q\mu_p\frac{\partial E_v}{\partial x} + qD_p\frac{\partial p}{\partial x}) \tag{8}$$

where $\varepsilon_0$ and $\varepsilon_r$ are the free space permittivity and the relative permittivity of the chlorophyll dye $\emptyset$ is the voltage profile, *x* is the dimension perpendicular to the cell surface, $J_n$ and $J_p$ are electron and hole current densities, *n* and *p* are electron and hole densities, $R_{n/p}$ is the electron and hole recombination rate, *G* is the generation rate, and $D_{n/p}$ is the diffusion coefficient. More detail on above equation resolving and device modelling can be found in more details in programme handbook from [14].

### *2.3 Device Structure and Simulation Parameters*

The basic design of an organic solar cells (OSC) is shown in Figure 2. The layer configuration adopted in this simulation is Glass / HTL / photosensitizers / electrolytes / ETL / Glass where the glass is the Fluorine Tin Oxide (FTO), the HTL layer is the Titanium Dioxide ($TiO_2$), the electrolytes layer is the potassium iodide (KI) and the ETL layer is the aluminium (Al) [15]. For this study, the chlorophyll-dye layer is set as an absorber layer which is a layer that allows photon absorption, charge separation and electrical conduction to the electrode. Therefore, Figure 3 describes the schematic representation which is the device structure of dye sensitized solar cell in GPVDM simulation.

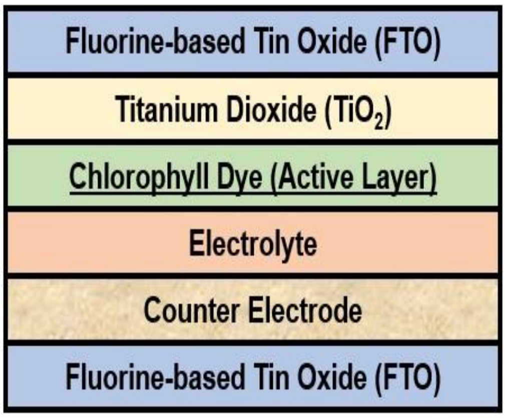


**Fig. 2.** Structure of developed DSSC

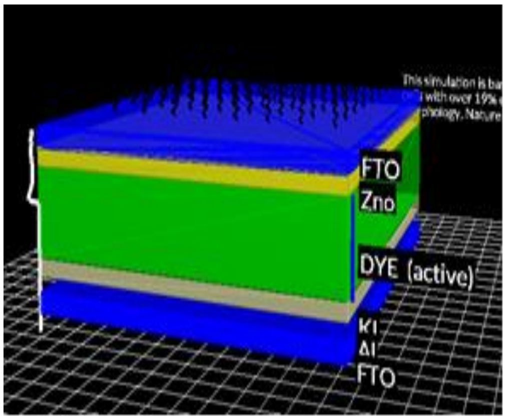


**Fig. 3.** Schematic view of DSSC in GPVDM

Next, the best option in this simulation is to use the default setting of all the related properties. This is because the most of the research paper does not mentioning or stated the electrical parameter of the organic cell. Hence, the electrical parameter and the other setting is set into default and expectable value to be used [16]. The simulation follows the exact size of active area DSSC that have been researched in previous research paper. Different types of chlorophyll dye are experimented on different size of conductive glass. The section to manipulate the size of DSSC in GPVDM software. Hence, it can follow the size that have been mentioned in published paper according to the type of chlorophyll dye. In Table 1 is summarized the design specification of electrical parameters for organic solar cell used for input configuration.

**Table 1**
List of electrical parameters in the GPVDM

| Electrical parameters | Values |
|---|---|
| Electron mobility | $2.48{\times}10^{-07}$ |
| Hole mobility | $2.48{\times}10^{-07}$ |
| Effective density of free electron states (@300K) | $1.28{\times}10^{27}$ |
| Effective density of free hole states (@300K) | $2.86{\times}10^{25}$ |
| Nfree to Pfree Recombination rate constant | 0.00 |
| Free carrier statistics | Maxwell Boltzman - analytic |
| Xi | 3.80 |
| Eg | 1.00 |
| Relatively permittivity | 3.80 |
| Substrate xz size | X = 0.0022804<br>Y = 0.0022804 |

## *2.4 Extraction of Material Data*

The material used in this simulation is the different dyes of chlorophyll. When the new absorber layer needs to be inserted into GPVDM software, the absorbance data and refractive index data are needed in order to run the simulation in it. All six samples of the new chlorophyll dye are inserted into GPVDM because the software does not have any data about the materials. Since the related data need to be acquired first, it is extracted from the previous research paper that have been experimenting of the chlorophyll dyes. The list of chlorophyll used is shows in Table 2 below.

**Table 2**
List of chlorophyll dye from previous article

| Author's name | Chlorophyll Dye | Area of photoelectrode ($cm^2$) |
|---|---|---|
| [17] | Azadiracha Indica (Chl A) | 2.25 |
| [18] | Prunus Armeniaca (Chl B) | 2.56 |
| [19] | Asimina triloba tree (Chl C) | 0.54 |
| [20] | Spinacia Oleracea (Chl D) | 0.25 |
| [21] | Cordyline fruitcosa (Chl E) | 1 |
| [22] | Ipomoea Purpurea (Chl F) | 0.25 |

### *2.5 Electrical Characteristics*

The current-voltage (I-V) and current density-voltage (J-V) characteristic can be produced by using the parameters that have been mentioned in subsection 2.3 and 2.4. The value of the y-intercept can be interpreted as the current short circuit (Isc) or current short circuit density (Jsc), while the x-intercept represents the open- circuit voltage (Voc) value. The current in the microamps unit is represented by the vertical on the left, while power in the microwatt unit is represented on the right. The voltage, measured in millivolts, is plotted along the horizontal axis of the graph. Figure 4 illustrates the perfect IV cell properties that would ideally exist. Figure 5 shown the current density-voltage in the GPVDM.

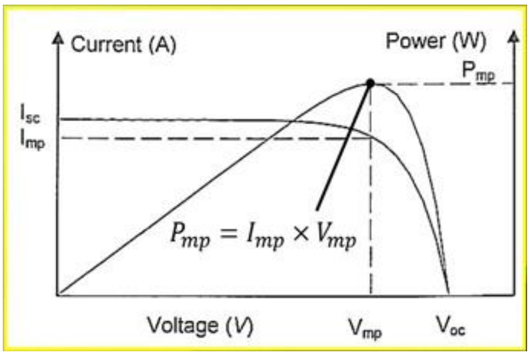


**Fig. 4.** The ideal of PV cell characteristics

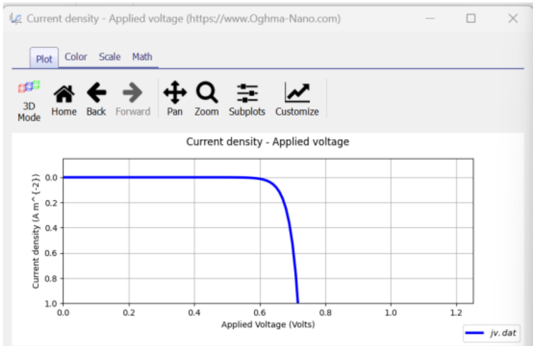


**Fig. 5.** J-V curve of Dye Sensitized Solar Cells

In this work, the short circuit current density is significant for comparing the findings to previous research. Hence, the comparison is performed by computing the MPE, or MPE difference, of Jsc. MPE is for mean percentage error, where SE stands for the experimental value of the quantity being predicted, SM stands for the prediction, and n stands for the variety of outputs for which the variable is predicted. The MPE equation is shown in Eq. 9. One way to evaluate the quality of a solar cell is to look at its fill factor. As indicated in Eq. 10 below, it can be determined by calculating the ratio of the Power maximum point (Pmp) divided by the Voc times the Isc value. When comparing the functionality of one solar cell to another, efficiency is the metric that is most frequently considered. It can be calculated by dividing the Power maximum point (Pmp) over irradiance of the light source (G) times the active area of $TiO_2$ (A). Eq. 11 provides a useful framework for describing it as follows

$$MPE = \frac{1}{n}\sum_{t=1}^{n}\frac{S_E - S_M}{S_M} \tag{9}$$

$$FF = \frac{Pmp}{Voc \times Isc} \times 100\% \tag{10}$$

$$\eta = \frac{Vmp \times Imp}{G \times A} \times 100\% \quad (11)$$

## 3. Results

### *3.1 Photovoltaic Performance of GPVDM*

DSSC performance is based on the output by simulation in GPVDM. All the chlorophyll dyes are inserted in GPVDM software and the significant parameter used for the dyes are absorbance and refractive index followed by previous paper. Thus, the result of simulation of I-V and J-V curve for six chlorophyll dyes is shown below and the value for simulation Isc, Jsc and Voc also tabulated below. The simulation follows the area of DSSC that have been mentioned in the related research paper.

#### *3.1.1 Azadiracha Indica leaves (Chl A)*

Figure 6 depicts the current-voltage (I-V) curve of the simulation using Azadiracha Indica leaves as the chlorophyll dye respectively. It can be observed from the curve that the result of short circuit current (Isc) is around 0.6 mA and the open-circuit voltage (Voc) is 0.5 V. Figure 7 shows the short circuit current-density (Jsc) is 0.2667 mA $cm^{-2}$.

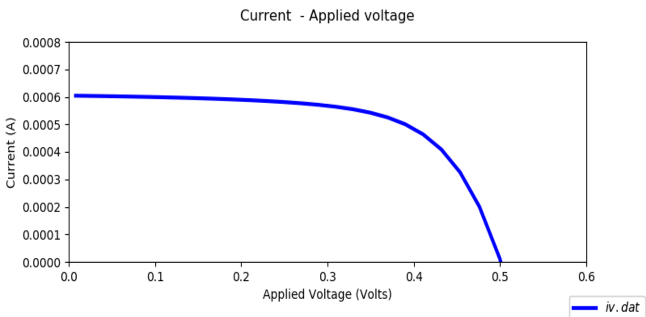


**Fig. 6.** The IV curve of Azadiracha Indica

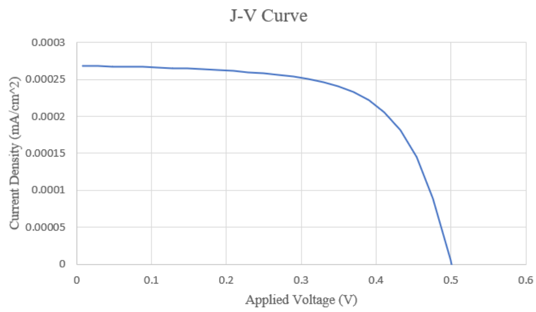


**Fig. 7.** The J-V curve of Azadiracha Indica

#### *3.1.2 Prunus Armeniaca (Chl B)*

The current-voltage (I-V) and the current density-voltage (J-V) curves of the simulation using Prunus Armeniaca leaves can be shown in Figure 8 and Figure 9. It can observe from the curve that the result of short circuit current (Isc) lies at around 0.695 mA and open-circuit voltage (Voc) lies at 0.524 V. The short circuit current density (Jsc) is lies at 0.271 mA $cm^{-2}$.

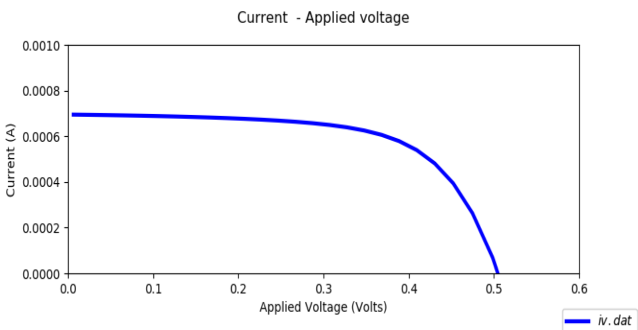


**Fig. 8.** The IV curve of Prunus Armeniaca Leaves

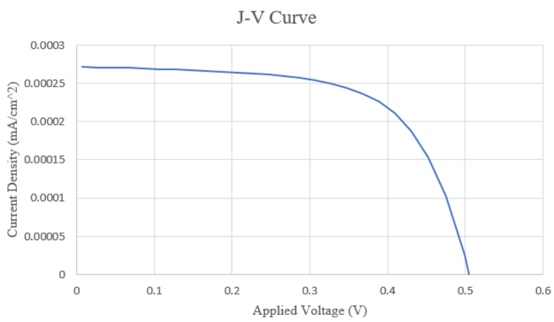


**Fig. 9.** The J-V curve of prunus Armeniaca leaves

### *3.1.3 Asimina Triloba leaves (Chl C)*

Figure 10 describes the current density-voltage (I-V) curve of the simulation using Asimina Triloba leaves. The short circuit current (Isc) lies approximately at 0.575 mA and the open-circuit circuit voltage (Voc) lies at 0.5 V. It can be observed from the curve that the result of short circuit current density (Jsc) lies at nearly 1.0648 mA cm$^{-2}$ as displayed in Figure 11.

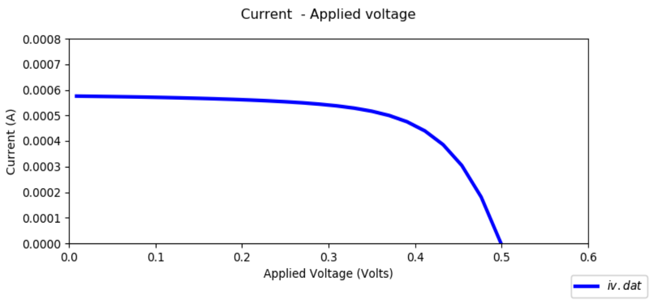


**Fig. 10.** The IV curve of Asimina Triloba Leaves

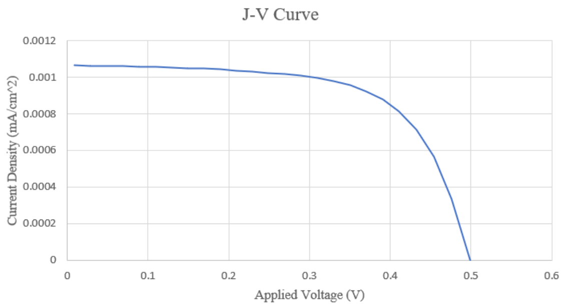


**Fig. 11.** The J-V curve of Asimina Triloba Leaves

### *3.1.4 Spinacia Oleracea leaves (Chl D)*

Figure 12 and Figure 13 depict the current-voltage (I-V) curve and the current density-voltage (J-V) curve of the simulation using Spinacia Oleracea leaves as dye respectively It can be observed from the curve that the result of short circuit current (Isc) is around 0.4 mA and the open-circuit voltage (Voc) is 0.479 V. Figure 13 shows the short circuit current-density (Jsc) is 1.6 mA cm$^{-2}$.

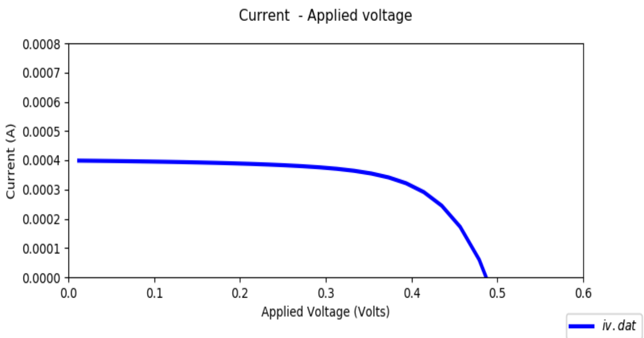


**Fig. 12.** The IV curve of Spinacia Oleracea Leaves

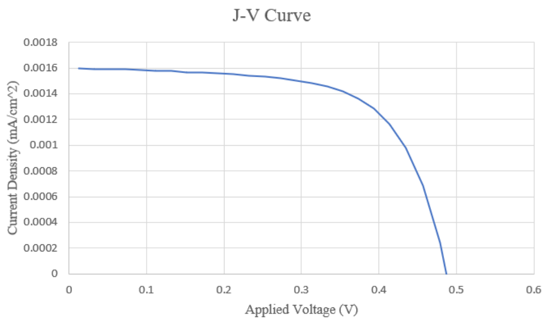


**Fig. 13.** The J-V curve of Spinacia Oleracea Leaves

### *3.1.5 Cordyline Fruticose leaves (Chl E)*

The current-voltage (I-V) and the current density-voltage (J-V) curves of the simulation using Cordyline Fruticose leaves can be shown in Figure 14 and 15. It can observe from the curve that the result of short circuit current (Isc) lies at around 0.8 mA and open-circuit voltage (Voc) lies at 0.523 V. Figure 15 shows the short circuit current density (Jsc) is lies at 0.8 mA cm$^{-2}$.

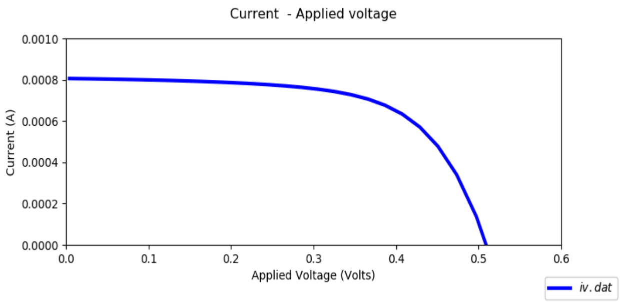


**Fig. 14.** The IV curve of Cordyline Fruticose Leaves

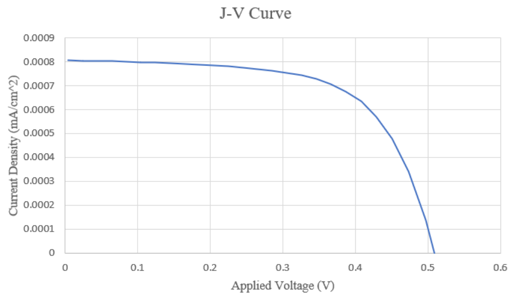


**Fig. 15.** The J-V curve of Cordyline Fruticose Leaves

### *3.1.6 Ipomoea Purpurea leaves (Chl F)*

The current-voltage (I-V) and the current density-voltage (J-V) curves of the simulation using Ipomoea Purpurea leaves can be shown in Figure 16 and 17. It can observe from the curve that the result of short circuit current (Isc) lies at around 0.287 mA and open-circuit voltage (Voc) lies at 0.48 V. Figure 17 shows the short circuit current density (Jsc) is lies at 1.148 mA cm$^{-2}$.

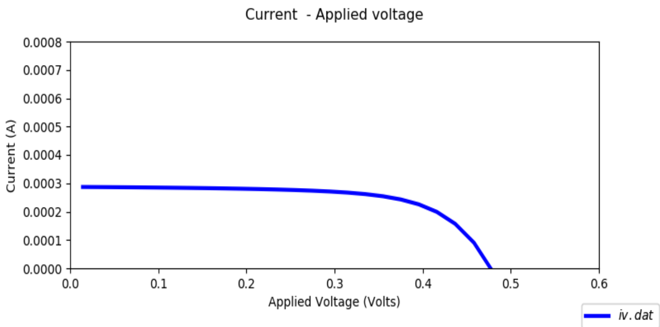


**Fig. 16.** The IV curve of Ipomoea Purpurea Leaves

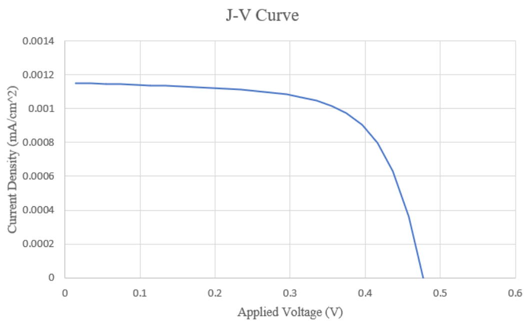


**Fig. 17.** The J-V curve of Ipomoea Purpurea Leaves

### *3.1 Discussion*

The summarized of the simulation result is being compared with the result of the previous research in the Table 3 and Table 4. From the six samples chlorophyll dye, Spinacia Oleracea (Chl D) dye shows the highest simulated value of short circuit current density (S Jsc) which is 1.6 mA cm$^{-2}$ compared to the research Jsc (R Jsc) and the others dye. Next, simulated value of open circuit voltage (S Voc), the Prunus Armeniaca (Chl B) dye shows the highest result with 0.524 V compared to the others dye.

**Table 3**
Comparison Between Research and Simulated Result of Short Circuit Current Density

| Chlorophyll | Area DSSC (cm$^2$) | R Jsc (mA/cm2) | S Jsc (mA/cm2) | MPE Jsc (%) |
|---|---|---|---|---|
| Chl A | 2.25 | 0.23 | 0.2667 | 15.96 |
| Chl B | 2.56 | 0.771 | 0.271 | -64.85 |
| Chl C | 0.54 | 0.649 | 1.0648 | 64.07 |
| Chl D | 0.25 | 1.11 | 1.6 | 44.14 |
| Chl E | 1 | 1.3 | 0.8 | -38.46 |
| Chl F | 0.25 | 0.85 | 1.148 | 35.06 |

**Table 4**
Comparison Between Research and Simulated Result of Open Circuit Voltage

| Chlorophyll | Area DSSC ($cm^2$) | R Voc (V) | S Voc (V) | MPE Voc (%) |
|---|---|---|---|---|
| Chl A | 2.25 | 0.467 | 0.5 | 7.07 |
| Chl B | 2.56 | 0.62 | 0.524 | -15.48 |
| Chl C | 0.54 | 0.504 | 0.5 | -0.79 |
| Chl D | 0.25 | 0.583 | 0.479 | -17.84 |
| Chl E | 1 | 0.616 | 0.523 | -15.10 |
| Chl F | 0.25 | 0.495 | 0.48 | -3.03 |

Meanwhile, the lowest difference for Jsc (MPE Jsc) and Voc (MPE Voc) is Chl A which is Azadiracha Indica leaves dye with 15.96 % and 7.07 %. This is due to the fact that when the mean percentage is used to compare the data from simulations and research, they are not significantly different. Therefore, it can state that the GPVDM simulation can be used to produce the same value. Then, another simulation has been conducted where all the size of active area of photoelectrode is assumed same which is 2.25 $cm^2$ and the result for simulated value of short circuit current (S Isc), short circuit current density (S Jsc) and open circuit voltage (S Voc) are tabulated in the Table 5. From six samples chlorophyll dye, Cordyline fruticose leaves (Chl E) dye shows the highest simulated value of short circuit current-density (S Jsc) which is 0.3556 mA/$cm^2$ compared to the others dye.

**Table 5**
Comparison of Simulated Result with Same Active Area of Photoelectrode

| Chlorophyll | Area DSSC ($cm^2$) | S Isc (mA) | S Jsc (mA/$cm^2$) | S Voc (V) |
|---|---|---|---|---|
| Chl A | 2.25 | 0.6 | 0.2667 | 0.5 |
| Chl B | 2.25 | 0.695 | 0.3089 | 0.524 |
| Chl C | 2.25 | 0.575 | 0.2556 | 0.5 |
| Chl D | 2.25 | 0.4 | 0.1778 | 0.479 |
| Chl E | 2.25 | 0.8 | 0.3556 | 0.523 |
| Chl F | 2.25 | 0.287 | 0.1276 | 0.48 |

## 4. Conclusions

In summary, this study conducts research on DSSC by finding the highest current-density (J-V) that can be produce from six samples chlorophyll dye by using General-purpose Photovoltaic Device Model (GPVDM) software. This software does not have sample structure of DSSC inside it, where we can use this software to identify the effectiveness of the software to simulate the dye-sensitized type solar cell.

From my observation, the highest simulated current-density (J-V) from six chlorophyll dyes that have been simulate for same active area is, Cordyline fruticose leaves (Chl E) with 0.3556 mA. Its value is the highest among other materials. The value of simulated short-circuit current-density (Jsc) are slightly difference to the value of experimented result Jsc from the published paper. It can be highly suggested that this GPVDM software is feasible to be used to simulate the DSSC structure.

As conclusion, this GPVDM can be considered as suitable for modelling the DSSC. However, mastering well in utilizing this software requires lots of effort and time since there are very limited sources available.

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