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Simulation and Performance of Natural Sensitizer Dye from *Lagerstroemia speciosa* Flowers and Leaves

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Authors' contributions

This work was carried out in collaboration among all authors. Author COO developed the statement of the problem, the route to follow as well as necessary tools to utilize, collated all the different sections, their arrangements and also proof read with major emphasis on the introduction and necessary references. The expanded abstract and conclusion was developed with authors AOB, BAI, SOO and ROK did the analytical calculations as well as the numerical simulations also author ROK wrote the introduction, reconfirm the analytical calculations and the numerical simulations and re-plotting where necessary. All authors read and approved the final manuscript.

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ABSTRACT

Dye-Sensitized Solar Cells (DSSCs) are solar cell devices that work using electrochemical principles in which sensitive dyes are absorbed in the titanium dioxide (TiO_2) photo-electrode layer. One of the key components of dye sensitized solar cells for developing high performance devices is the dye, which acts as the photosensitizer. However, using natural dyes from plant sources has produced low power conversion efficiency (PCE) compared to organic synthetic dyes. In this study, the performance of locally extracted dye from *Lagerstroemia speciosa* leaves and flowers has been determined by simulation using MATLAB based on TiO_2 by modifying the internal parameters such as the absorption coefficient and diffusion coefficient, external, and previous DSSC research data. The simulation produced a high-power conversion efficiency and current density of 1.82% and 14.32 mA/cm^{-2} respectively. The results obtained from the simulation shows that this plant can be used as photosensitizers in DSSCs in the future.

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1. INTRODUCTION

Energy is essential for the development of mankind. Also, the advancement in technology and growth of population have resulted in the need for alternative sources of energy from fossil fuels. This has led into the discovery of photovoltaic devices which enable us to convert solar energy from the sun into electricity. Dye sensitized solar cells (DSSCs) represent a new generation of solar cells which are less expensive to fabricate, and uses natural dyes from plants for the generation of electricity. DSSCs is based on nano-porous titanium dioxide (TiO_2) films which have been broadly researched due to their comparable photovoltaic efficiency, potentially low production cost, low toxicity, and rapid manufacturing process. Also, the advantages of DSSCs for real-world applications, including transparent and multicolor options, or both, easy architectural integration, and short energy payback time have drawn attention [1,2]. The general DSSC consists of a dye-adsorbed semiconductor electrode (i.e., TiO_2 or zinc oxide (ZnO) photo electrode), an electrolyte and a platinum (Pt) or carbon-coated counter electrode [3, 4]. The photo electrodes in the device play an important role in the photovoltaic efficiency. Highly porous photo electrode films provide extended surface area for dye adsorption resulting in the enhanced light harvesting efficiency (LHE) of DSSCs. When the material molecules absorb sunlight the electrons transition from the ground state to the excited state.

A continuity equation of dye sensitized solar cell (DSSC) was established based on the diffusion theory of electron transport. Using the internal parameters suitable of titanium dioxide (TiO_2) as photo-anode, the internal mechanism affecting DSSC electron injection and transmission was studied [5]. The factors affecting the photoelectric properties of DSSC, such as temperature, TiO_2 film thickness, electron lifetime, electron diffusion coefficient, light intensity and absorption coefficient, were studied respectively.

The problem of Dye-Sensitized Solar Cell is the efficiency that is still low compared to silicon solar cells [6]. The efficiency of DSSC uses natural dyes about 12.3% [7], while the efficiency of silicon solar cells is approximately 20% [8]. Low efficiency is due to a high levelof recombination of free electrons with oxidized dye molecules [9]. One that causes high levels of recombination is the limitation of electron transfer in TiO_2 layers. The low transfer of electrons is due to less optimal contact between particles. Low electron transfer will cause electrons to be trapped at the boundary between TiO_2 particles. Furthermore, electrons trapped at this grain boundary result in higher recombination opportunities [10]. The use of combination of natural red and green dyes to improve the power conversion efficiency of dye sensitized solar cells was also report in [11-14]. Extensive research on improving the PCE of DSSCs based on different natural and synthetic dyes have been conducted since the first report on dye-sensitized, but little attention has been given to the use of simulation to first determine the efficiency of the extracted dye samples. To the best of our knowledge, simulation DSSCs have rarely been reported. In this study, the absorbance simulation of *Lagerstroemia speciosa* dye extracts would be investigated to determine its photovoltaic parameters of the extracted samples.

2. METHODOLOGY

2.1 Extraction of Dye

Lagerstroemia speciosa leaves and flowers were collected within the campus of Lagos State University, Ojo, Nigeria. The samples (flowers and leaves) were air dried at room temperature for 4 hours. With the aid of liquidizer, the samples were pulverized. The pulverized samples were soaked separately using a solvent system that comprised of distilled water, methanol and concentrated HNO_3 in ratio 10: 9: 1, respectively. The sample was filtered and the filtrate represents the crude sample. Using the method of [15], the anthocyanin was obtained from the sample. The absorbance of the extracted samples was carried out using the ultraviolet-visible spectrophotometer. The crude and purified extracts for the flowers and leaves are represented as: crude extract for leaves and flower (D1 L and D1 F) and purified extracts for leaves and flower (D2 L and D2 F) respectively.

2.2 Theoretical Simulation

Theoretically the photo-electrochemical behavior in the DSSC photo-electrode nanostructure was analyzed using the method Soedergren et al. [16]. The resulted equation relates the electron transport, electron recombination, and electron photo-generation in thin films DSSC as:

$$D\frac{\partial^2 n(x)}{\partial x^2} - \frac{n(x)-n_o}{\tau} + \emptyset_o \alpha exp(-\alpha x) = \frac{\partial n}{\partial t} \quad (1)$$

Where $n(x)$is the number of excessive electrons photo-generation concentrations at position x in the photo-electrode interface layer, n_o represents concentration of electrons below the equilibrium of the dark conditions, D correspond to the diffusion coefficient of the electron. The parameters τ, $\emptyset_o$ and α represent the lifetime of the free electrons in the conduction band, the intensity Flux illumination of photons and light absorption coefficient of the thin film. In this paper, the internal parameters in the DSSC (Φ, α, m, L, D) from previous researches which are written in Table 1 was used for the simulation [17].

The simulation activity was done with the input of DSSC equation in m-file in MATLAB along with the absorption coefficient of each of the extracted dye. The equations related to the simulation model are as follows:

$$J_{sc} = \frac{q\emptyset L\alpha}{1-L^2\alpha^2}\left[-L\alpha + tanh\left(\frac{d}{L}\right) + \frac{L\alpha exp(-d\alpha)}{cosh\left(\frac{d}{L}\right)}\right] \quad (2)$$

$$V_{oc} = \frac{KTm}{q} ln\left[\frac{LJ_{sc}}{qDn_o tanh\left(\frac{d}{L}\right)} + 1\right] \quad (3)$$

$$J = J_{sc} - \frac{qDn_o}{L}\tanh\left(\frac{d}{L}\right)\left[exp\left(\frac{qv}{KTm}\right) - 1\right] \quad (4)$$

3. RESULTS AND DISCUSSION

The absorbance of the dye extracts is shown in Fig. 1. It is observed that the purified flower extract exhibits a higher absorption in comparison to other dye extracts. Consequently, the low absorption obtained for the leaves extract (D1 and D2) is attributed to compounds in the extract which inhibit the absorption of light or low level of anthocyanin. Also, the current density (J_{sc}), open circuit voltage (V_{oc}) and power conversion efficiency (PCE) was measured through simulations for the extracted dye samples. The analysis was done based on equation 2, which describes the photochemical behavior of DSSCs. The effect of the absorbance of the extracted dyes on the photovoltaic parameters is shown in Fig. 2 to 5 and Table 2. It is observed from Table 2, that purified flower extract provides the highest PCE. This increase in PCE compared to other extracts can be attributed to the removal of other compounds in the dye which inhibit the absorption of light. The reduction in PCE for the crude and purified leave extracts can be attributed to the absorbance coefficient of the dye which is proportional to the magnitude of the voltage and current density obtained [18]. Also, the simulation of high absorption coefficient of dye extracts improves the performance of DSSCs as observed in the crude and purified flower extracts [19,20] that a high concentration of anthocyanins in the extracts leads to low photovoltaic performance which was observed during the simulation.

Table 1. Simulation parameters

Parameter	Published value
L ($cm^{-1}s^{-1}$)	2.2361×10^{-3}
$\boldsymbol{\alpha}$ (cm^{-1})	5000
M	4.5
D (cm^{-1} s^{-1})	5.0×10^{-4}
$\boldsymbol{n_0}$	10^{16}
$\boldsymbol{\tau_{ms}}$	10
∅ (cm^{-2} s^{-1})	1.0×10^{17}
d (cm)	10×10^{-4}
T (K)	300

Table 2. Photovoltaic parameters for the simulated dye extracts

Sample	J_{sc} (mA/cm^2)	V_{oc} (mV)	PCE x 10^{-3} (%)
D1 F	9.55	0.65	1.21
D1 L	5.59	0.32	0.07
D2 F	14.32	0.69	1.82
D2 L	3.78	0.27	0.04

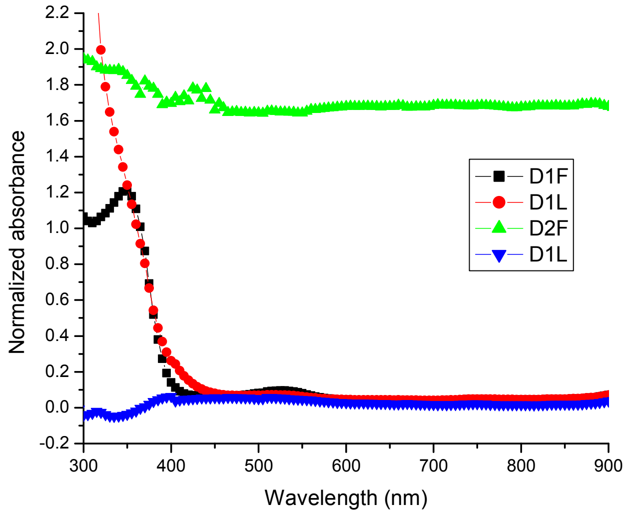

Fig. 1. Absorbance of extracted dye

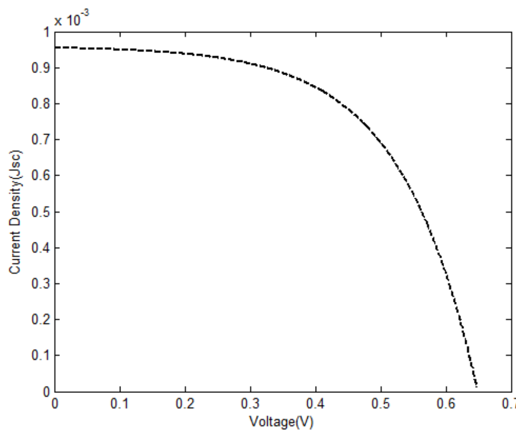

Fig. 2. Simulation for crude flower extract

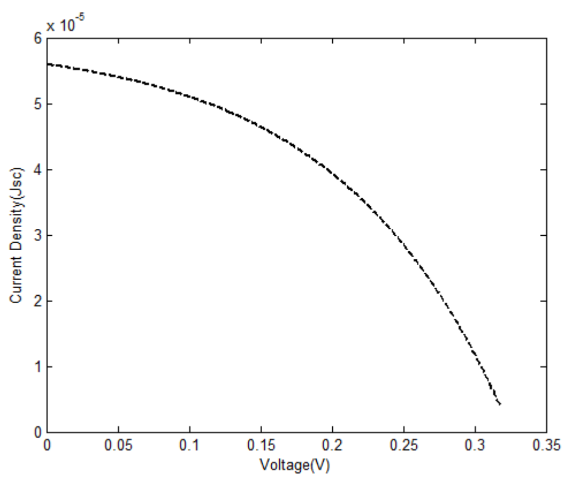

Fig. 3. Simulation for crude leaf extract

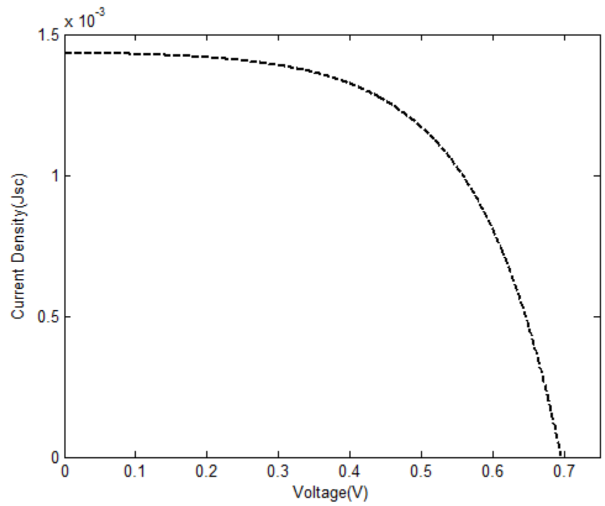

Fig. 4. Simulation for purified flower extract

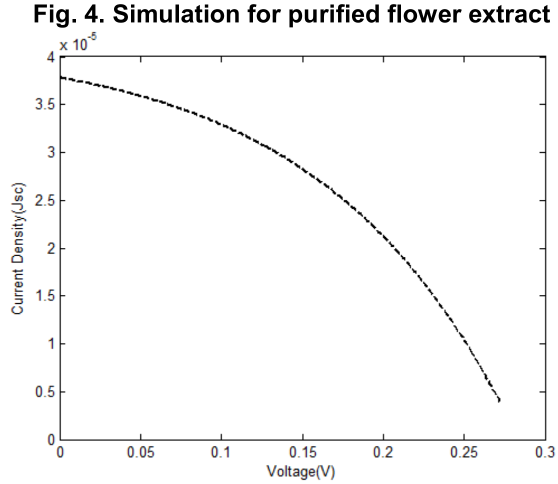

Fig. 5. Simulation for purified leaf extract

4. CONCLUSION

This simulation is performed to determine the performance of DSSCs using the theoretical method based on internal parameters and factors that enhance the performance of DSSC. This method is based on analyzing photo-electrochemical behavior on DSSC centered on photo-electrode electron diffusion process so that the value of current density (Jsc), open circuit voltage (Voc), and power conversion efficiency are obtained. The analysis was performed based on one of the factors influencing DSSC performance which is the absorption coefficient. This study still needs further development by adding other existing parameters as well as external factors to the DSSC to match the experimental values. Also, in order to improve the performance of DSSC, a combination of different dyes should be applicable.

COMPETING INTERESTS

Authors have declared that no competing interests exist.

REFERENCES

1. Freitag M, Teuscher J, Saygili Y, Zhang X, Giordano F, Liska P, et al. Dye-sensitized solar cells for efficient power generation under ambient lighting. Nature Photonics. 2017;11(6):372-378.
2. El Tayyan AA. Dye sensitized solar cell: Parameters calculation and model integration, Journal of Electron Devices. 2011;11:616-624.
3. Adenike B, Okafor P, Ibrahim A, Oluwole S, Boyo H. Application of *Hibiscus sabdariffa* and leaves of *Azardirachta indica* calyxes as sensitizers in Dye-

sensitized solar cells, International Journal of Engineering Research and Development. 2013;8(12):38-42.
4. Boyo A, Oseni O, Ibrahim O, Kesinro R, Akingbade F, Oladepo A et al. Performance simulation of *Ipomoea involucrata* dye extracts for dye sensitized solar cells. Journal of Energy Research and Reviews. 2020;30-39.
5. Kingsley JW, Green A, Lidzey DG. Fabrication and optimization of P3HT: PCBM organic photovoltaic devices. 74160T.
6. Nazeeruddin MK, Baranoff E, Grätzel M. Dye-sensitized solar cells: A brief overview. Solar Energy. 2011;85(6):1172-1178.
7. Arifin Z, Soeparman S, Widhiyanuriyawan D, Purwanto A, Dharmanto. Synthesis, characterisation, and fabrication hollow fibres of Zn-doped TiO2 for dye-sensitized solar cells. Journal of Engineering Science and Technology. 2017;12(5):1227-1239.
8. J. Perlin. From space to earth: the story of solar electricity: Earthscan; 1999.
9. Hara K, Horiguchi T, Kinoshita T, Sayama K, Sugihara H, Arakawa H. Highly efficient photon-to-electron conversion of mercurochrome-sensitized nanoporous ZnO solar cells. Chemistry Letters. 2000; 29(4):316-317.
10. Yu H. Modification of TiO2 photoanodes for dye-sensitized solar cells: Griffith University; 2011.
11. Bashar H, Bhuiyan MMH, Hossain MR, Kabir F, Rahaman MS, Manir MS, Ikegami T. Study on combination of natural red and green dyes to improve the power conversion efficiency of dye sensitized solar cells. Optik. 2019;185:620-625.
12. Rajabi HR, Arjmand H, Kazemdehdashti H, Farsi M. A comparison investigation on photocatalytic activity performance and adsorption efficiency for the removal of cationic dye: quantum dots vs. magnetic nanoparticles. Journal of Environmental Chemical Engineering. 2016;4(3):2830-2840.
13. Cheng You-liang, Wei-ping Y. Numerical simulation of electron transmission of dye-sensitized solar cells. Advances in N and R Energy. 2020;8(1):68-74.
14. Richhariya G, Kumar A, Tekasakul P, Gupta B, Natural dyes for dye sensitized solar cell: A review. Renewable and Sustainable Energy Reviews. 2017; 69:705-718.
15. Taofeek AO, Salawu NA, Yakubu MT, Oladiji AT, Akanji MA, Okogun JI. Antioxidant and drug detoxification potentials of *Hibiscus sabdariffa* anthocyanin extract. Drug and Chemical Toxicology. 2011;34(2):109-115.
16. Soedergren S, Hagfeldt A, Olsson J, Lindquist S-E. Theoretical models for the action spectrum and the current-voltage characteristics of microporous semiconductor films in photoelectrochemical cells. The Journal of Physical Chemistry. 1994;98(21):5552-5556.
17. Habieb AM, Irwanto M, Alkian I, Sya'diyah FK, Widiyandari H, Gunawan V. Dye-sensitized solar cell simulation performance using MATLAB. 1742-6596.
18. Supriyanto E, Kartikasari HA, Alviati N, Wiranto G. Simulation of Dye-Sensitized Solar Cells (DSSC) Performance for Various Local Natural Dye Photosensitizers. 012048.
19. Syafinar R, Gomesh N, Irwanto M, Fareq M, Irwan Y. Chlorophyll pigments as nature based dye for dye-sensitized solar cell (DSSC), Energy Procedia. 2015;79:896-902.
20. Godibo DJ, Anshebo ST, Anshebo TY. Dye sensitized solar cells using natural pigments from five plants and quasi-solid state electrolyte. Journal of the Brazilian Chemical Society. 2015; 26(1):92-101.

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