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A dye-sensitized solar cell model implementable in electrical circuit simulators

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Abstract

The main goal of the present work is to provide a mathematical model of Dye-Sensitized Solar Cells (DSCs) that can be implemented in electrical engineering circuit simulation software, such as PSIM, for using in electronic power converter design. Consequently, a new circuit modeling approach is presented, able to solve the standard continuity and transport governing equations defined for the involved mobile species: electrons in the TiO_2 conduction band and ions in the electrolyte. Starting from the partial differential continuity equations of the phenomenological DSC model, it was developed a one-dimensional spatial discretization using Finite Difference Methods (FD) followed by a solution using an electrical circuit analogy. The resulting circuits were then implemented in PSIM software and simulated. Simulation results using this new electrical analog approach showed excellent matching when compared to FORTRAN numerical solutions, as well as when compared to experimental data. Moreover, the electrical analog can be used for transient and steady state cases, giving information about the main factors and the relevant kinetic parameters that influence DSCs' performance. Finally, it enables to relate the phenomenological behavior with other electrical approaches, such as Electrochemical Impedance Spectroscopy (EIS) and diode based models.

Keywords: Dye-sensitized solar cells; Modeling and simulation; *I–V* characteristics; PSIM; Finite differences

1. Introduction

Dye-Sensitized Solar Cells (DSCs) are a third generation of photovoltaic technology formed by a combination of organic and inorganic components that can be produced at very low cost. DSCs consist of a porous nanocrystalline TiO_2 layer deposited onto a transparent conducting oxide (TCO) glass substrate and coated with a monolayer of dye. Under illumination, the dye absorbs the radiation and, once excited, electrons are injected into the conduction band of TiO_2. The photoinjected electrons then percolate through the semiconductor network, being collected at the TCO. Following electron injection, oxidized dye molecules are regenerated by electron donation from the electrolyte solution containing a redox couple of iodide/triiodide. The triiodide ions formed on the semiconductor's surface during the redox reaction diffuse to the platinum-catalyzed counter-electrode (CE), where they are reduced back to iodide by the electrons from the external circuit (Grätzel, 2000, 2009; Andrade et al., 2010).

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Nomenclature

A	cell area, m^2
C_i	concentration of species i, M
D_a	dimensionless number (equivalent to Damkolher number)
D_i	diffusion coefficient of species i, $m^2\ s^{-1}$
D_{ref}	reference diffusion coefficient, $m^2\ s^{-1}$
E	energy, J
E_{cb}	conduction band energy, J
E_{redox}	redox energy, J
E^0_{redox}	standard redox energy, J
E^{oc}_{redox}	open circuit redox energy, J
FF	fill factor
G_i	generation rate of specie i, $m^{-3}\ s^{-1}$
h	spacing size of the nodes
I	electric current, A
I_s	incident photon flux, $m^2\ s^{-1}$
j	node
j_i	current density of species i, $A\ m^{-2}$
j_0	exchange current density at the counter electrode, $A\ m^{-2}$
k	maximum number of nodes
k_B	Boltzmann constant, $J\ K^{-1}$
L	thickness of the TiO_2 film, m
n_i	density of species i, m^{-3}
n_{eq}	dark equilibrium electron density, m^{-3}
n_{ref}	reference particle density, m^{-3}
N_{CB}	effective density of states in the TiO_2 conduction band, m^{-3}
q	elementary charge, C
R_i	recombination rate of species i, $m^{-3}\ s^{-1}$
R_p	shunt resistances, Ω
R_{series}	external series resistances, Ω
R_c	contact and wire series resistances, Ω
R_{TCO}	transparent conductive oxide sheet resistance, Ω
R_{ext}	load parameter: external resistance, Ω
T	temperature, K
t	time, s
V_{ext}	external cell potential, V
V_{int}	internal cell potential, V
V_{oc}	open-circuit potential, V

Greek letters

$\alpha(\lambda)$	wavelength-dependent absorption coefficient, m^{-1}
β	recombination reaction order
α	symmetry coefficient
γ	dimensional number
ΔV_{int}	variation of the applied potential, V
ΔV_{cb}	shift in the conduction band potential, V
ε	porosity of the TiO_2 film
η_{Pt}	electrochemical overpotential at Pt electrode, V
η_{inj}	electron injection efficiency
θ	dimensionless time variable
λ	wavelength, m
τ_{e-}	electron lifetime, s
ϕ	dimensionless number (equivalent to Thiele modulus)

Superscript

*	dimensionless variable
0^+	xx coordinate close to the photoanode
0^-	external point of the current collector
init	initial conditions

Subscripts

c^+	cations
CB	conduction band
CE	counter electrode
e^-	electrons
I^-	iodide
I_3^-	triiodide
MPP	maximum power point
OC	open circuit
SC	short-circuit
STC	standard test conditions
TCO	transparent conductive oxide

DSCs offer the prospect of a cheap and versatile technology for large-scale production of solar cells. In terms of energy generation, DSCs are able to efficiently convert both direct and diffuse light and so they are able to absorb the non-perpendicular incident solar radiation, eliminating the need of complex sun tracking systems, with a minimal energy efficiency loss. DSCs start producing electricity earlier in the day and finish later, being highly adaptable to cloudy weather and room lighting. They are less sensitive to temperature, enabling a stable efficiency for a temperature range up to 80 °C, unlike silicon technologies that strongly decreases the efficiency with temperature. DSCs can be made semi-transparent, with various possibilities of colors and diverse patterns, being pleasant. Finally, these devices are easily scalable to large size cell applications and spend less energy during the manufacturing process than conventional PV technologies, making them an environmentally friendly product (Hodes, 2013; Park, 2013; Boix, 2014).

In order to improve DSCs performance and optimization, detailed physical models based on diffusion, recombination and charge transport phenomena have been developed to illustrate its operation (Andrade et al., 2011; Maçaira et al., 2014; Soedergren et al., 1994; Bisquert and M-Seró, 2010; Kalyanasundaram, 2010; Wang et al., 2006). These are accurate mathematical models that describe DSCs behavior by means of partial differential equations (PDEs) in space and time. However, the software