Minimisation of the cost of generated electricity from dye-sensitised solar cells using numerical analysis

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Abstract

Arrays of thin-film solar cells based on dye-sensitised nanocrystalline oxides (DSC) promise low-cost electricity especially where continuous direct insolation is unavailable. However, the optimisation of arrays of DSC is not straightforward because of the lower power levels obtained and the corresponding increased stringency needed when calculating the production tolerances permissible in the individual cells. This paper describes the first stage of project to devise and build a DSC array simulator driven solely by a phenomenological model of individual DSC behaviour at the level of infinitesimal cells. The simulator numerically extrapolates this behaviour to real finite cells and thence to a real physical array. In the process it is observed that optimisation of infinitesimal cells is only possible when the size of the real cell is first decided, and that the relationship between the conducting oxide transparency and electrical resistance is critical for the optimisation to be effective. The results obtained using the simulator are compared with the behaviour of real test cell assemblies manufactured by STI, a DSC Licensee, and are found to be in good agreement. Their effects on the costs of delivered power are discussed.

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1. Introduction

The cost of electricity generated by a renewable resource is a critical figure used by investors when deciding whether to proceed with a particular project in which renewable energy could play a role. It is practically more important than the efficiency of conversion of solar energy into electricity, which is the parameter commonly subjected to maximisation by researchers. The cost of generated electricity depends the cost of the cell array, which in turn depends on a number of sensibly independent factors, not all of which feature in setting the efficiency of the product. They include:

- number of production processes used;
- length of time processes need to run;
- accuracy to which process parameters need controlling;
- purchase costs of raw materials.

The efficiency of the product is also related to the above, but with one extra parameter:

- The settings of the production process parameters.

It is therefore possible to alter the cost of generated electricity by adjusting process parameters at little or no marginal cost, and achieve significant variations in the efficiency of the product, and hence the cost of electricity generated.

Other factors which will be considered in later work include the lengths of time over which the solar array is exposed to sunlight of a particular intensity. The ability of PV cells to generate electricity in low light, and under diffuse irradiation, allowing fixed mounting, may lead to cheaper long-term energy generation than more efficient cells which only operate under high irradiation, but do not work well under the majority of conditions faced by the array. Silicon technology suffers from this drawback, while CIS is even worse and generates no significant power in less than full sun due to its propensity to substantial shunt conductance pathways across the cells.

This paper examines dye-sensitised solar cells and arrives at a design criteria for optimising their operation. The effect on the cost of generated electricity is discussed.

Silicon semiconductor technology has made it possible to construct solar cells of good performance for connection in arrays by means of, usually, metallic wires strung between individual cells. This procedure is labour intensive, and does not readily permit fully automated assembly of large solar cell arrays [1]. This issue, combined with the cost of solar cell grade silicon, has resulted in much effort being devoted in recent years to the design and construction of solar cells based on thin and thick film technologies. A particularly promising embodiment of thin film cells is the use of a dye-sensitised semiconductor, usually a metallic oxide, fabricated on a conducting substrate, or between two conducting substrates, where at least one of the substrates is optically transparent [2]. In the conventional approach the
substrates comprise glass coated with a transparent electronic conductor. Recently new designs based on flexible light weight substrates (e.g. polymeric and/or thin metal foil) have been introduced [3], though efficiencies are yet to rival inorganic designs. The presence of a transparent electrical conductor (e.g. transparent conducting oxides or fine metallic mesh) is a common feature of DSCs.

Abandoning the use of wires to interconnect DSCs has considerable implications on cell performance. The cell-to-cell resistance and the resistance between the individual elements of a single cell are no longer negligible [4], and become largely responsible for the difficulty in efficiently removing power from such cells in real assemblies. The harder it is to remove the power, the less likely it is that the ultimate output energy will be inexpensive.

Many groups have reported investigations into the internal operation of DSCs, with a good overview of current state of the art research by McConnell [5]. Such work, excellent though it may be, typically fails to consider the one single parameter which a typical user would rely on to select cells of one design over another—the cost of the electricity generated. Concentration on related, but non-defining factors such as cell efficiency can lead researchers along less advantageous pathways which serve to dissipate their efforts on optimising irrelevant parameters. It is the purpose of this research to bring the focus of DSC development back to earth and demonstrate what has to be achieved, and how, to enable these devices to be made and used profitably.

The research presented in this paper is therefore driven by the need to thoroughly simulate potential systems together with the expected losses, so that the design of the assembled array can be chosen to provide the most cost-effective energy that the technology can provide.

In this study the interaction between the cell conductive oxide thickness, conductive oxide transparency, light level and size were investigated with the aim of optimising cell performance without increasing cell costs. Such an optimisation was recognized to be likely to result in different combinations of cell parameters which provided for maximum output depending on the intensity of the incident solar energy. Future studies will investigate the performance of arrays using various types of cell physical interconnections, with alternative topologies, and with different areas of the cell committed to interconnections.

Such an investigation has been undertaken with silicon cells, especially those used in concentrator applications, where similar trade offs between collector track width and cell exposure need to be made [6]. To date, however, this approach has not been reported for DSC. In this paper we report on an optimisation process developed using a standard electronic circuit emulator (MicroCap) to analyse the behaviour of a real cell, under varying conditions, and determine by numerical analysis the optimum thickness for the conducting films in different situations. Given some estimated cost parameters for DSC arrays, it is then possible to demonstrate how the price of generated power from a real array varies with individual cell design. In the next stage, shadowing of the array will be accommodated, as has been done for silicon systems by Woyte et al. [7].
2. Model

A real cell (a cell of finite dimensions and with finite transverse ohmic losses) is modelled by decomposing it into short “elemental cells” of negligible transverse ohmic losses, which are then connected in transmission line fashion including small inter-element resistances to emulate a complete cell.

2.1. Elemental cell

Such an elemental cell is not a real construct but a mathematical concept. It can nevertheless be simulated sufficiently close by a small enough cell with correspondingly low transverse ohmic losses attributable to the conducting film on which the cell is constructed.

The design of such an elemental cell must reflect the actual structure and operation of DSC, but with appropriate simplifications and approximations required to create a model within the circuit simulator. Fig. 1 schematically shows the working principles of dye-sensitised titania solar cells [8–12].

Incident light is absorbed by the photosensitive dye molecules in their ground state (S) and the molecules are excited to a new state (S*). The excited molecules inject electrons into the conduction band of the TiO₂, and thus become ionised (S⁺). This corresponds to the generation of a photocurrent (I_photo). In a perfect cell I_photo would be exactly proportional to the incident illumination, but in real cells a non-linearity is observed.

TCE represents the transparent conductive electrode on the positive and negative terminals of the cell. On the negative electrode the electrons encounter an effective

![Fig. 1. The structure of elemental cell, showing the working principles of the DSC (see text).](image-url)
resistance, $R_T$ representing the series resistance of the TCE plus the titania. On the positive electrode the electrons encounter an effective resistance $R_{\text{elyte}}$ representing the series resistance of the electrolyte plus the TCE.

The electrons diffuse through the TiO$_2$ to the TCE and work is done through an external load (connected across $V^+ - V^-$), thereby yielding usable energy. The electrons then move to the platinum catalysed counter electrode (deposited on the TCE) where they reduce the redox species present ($R \rightarrow R^-$). The reduced ions are subsequently transported through the electrolyte solution ($R_{\text{elyte}}$) and eventually contact the ionised dye molecules. The ionised dye is then reduced by the redox species ($R^- \rightarrow R$) thus returning it to its original state and completing the circuit.

There is an alternate pathway for the electrons to return to the S state of the dye. They may fail to exit the cell and recombine directly with molecules in the electrolyte, effectively shunting the cell with a current $I_{\text{sh}}$ proportional to an exponential function of the potential between the titania bandgap and the higher level of the couple. This phenomenon is observed in some form in all semiconductor cells and is a major source of energy loss, manifesting as a severe limit on the cell voltage, and hence power output.

The energy level of the S* state of the dye is higher than that of the conduction band of the titania by a value $V_{bg}$, which contributes a further minor but non-negligible source of loss. This is because the full energy of the incident photon is not transferred to the photoelectron in the titania conduction band, some being lost through phonon creation as the electron falls from the S* state.

The electrical equivalent circuit utilised for simulation of this elemental cell is presented in Fig. 2.

The entire cell element could have been readily modelled by a two-dimensional table relating current through the cell with voltage across it and insolation incident upon it, had this been readily available in the software simulator. In this approximation, an equivalent circuit was used, as illustrated in Fig. 2. Each element

![Equivalent circuit of cell element](image)

Fig. 2. Equivalent circuit of cell element. $R_{\text{elyte}}$—effective ohmic resistance of electrolyte, $R_T$—effective ohmic resistance of titania, $I_{\text{photo}}$—photocurrent, determined by illumination, $I_{\text{sh}}$—Shunt current caused by recombination.
in the equivalent circuit can be related to a key component of the actual DSC, as discussed below.

The photocurrent $I_{\text{photo}}$ in mA was modelled using an empirically determined non-linear expression relating it to sun level $I_{\text{ill}}$:

$$I_{\text{photo}} = 0.84I_{\text{ill}} - 0.193I_{\text{ill}}^2,$$

where the coefficients are appropriate for a cell of 0.05 cm$^2$.

The recombination current $I_{\text{sh}}$ was accommodated by using a non-linear voltage-to-current converter, which shunted a current from the cell positive to the cell negative electrodes via the electrolyte. The behaviour of such electrochemical junctions under these conditions has been analysed by many workers [13,14], and it is generally recognised that current $I_{\text{sh}}$ versus voltage $V_d$ characteristics of such an element are conveniently represented in simplified form by that of a diode element

$$I_{\text{sh}} = I_0 \exp \left( \frac{AV_d}{kT} \right),$$

where $I_0$ is a constant conventionally known as the diode saturation current, $k$ is Boltzmann’s constant, $T$ is the temperature in K, and $A$ is a constant dependent on the diode material and geometry.

In the case considered here, and assuming a cell size of 0.05 cm$^2$ as an example, the expression can be expressed numerically as

$$I_{\text{sh}} = 6.5 \times 10^{-13} \exp(30V_d) \text{ in amps},$$

The cell size chosen as an example here of 0.05 cm$^2$ also matches that of the size selected later in the research as particularly convenient for an elemental cell.

A voltage source originating elsewhere in the external circuit represented the sunlight reaching the dye after absorption in the conducting film. The bandgap voltage mismatch, being in series with a current generator, was of no significance in this simulation and was ignored for the remaining simulations. Charge transfer resistance at the counter electrode was included in $R_{\text{lyte}}$. Overpotential at the counter electrode was neglected in this approximation. Finally, in order to simulate reverse bias conditions, the recombination element was defined as reversible to shunt electrons from the electrolyte to the titania when the titania became more positive than the electrolyte.

A critical step in simulating a cell accurately accounts for the reduction in light intensity reaching the dye as more conductive, but more opaque, TCE films are used. As the film resistivity is lowered, the thickness of the oxide layer in the TCE increases and the light transmission $T$ decreases according to the theoretical relationship

$$T = I \exp(-\alpha t),$$

where $I$ represents the incident radiation, $\alpha$ is the average absorption coefficient of the TCE over the spectral range in question and $t$ represents the thickness. It is assumed that $\alpha$ is independent of film thickness, although for some thin films this might not be the case, since it comprises components of absorption, internal scattering, and reflection. The first depends only on thickness, the second may vary as a power of thickness and the third will be constant. For plain, clear float glass, the
transmittance $T_{\text{glass}}$ is related to the reflectance $R_{\text{glass}}$ by

$$T_{\text{glass}} = (1 - R_{\text{glass}}).$$

When a film of thickness $t > 0$ is deposited on the glass the film itself will have a reflectance $R_{\text{film}}$ which replaces the value $R_{\text{glass}}$ in Eq. (5). The formula for overall transmittance $T$ therefore becomes, from Eqs. (4) and (5)

$$T = (1 - R_{\text{film}}) \exp(-zt)$$

valid for $t > 0$ (not for $t \geq 0$). The combination of glass transparency (~0.92, typical) and film reflectance (~0.09 typical) causes Eq. (4) to show an asymptote at 0.835, and not 0.92 as may be expected from clear glass.

Pilkington gives a number of discrete values of transmittance and corresponding sheet resistance in the material data sheet [15]. Fitting these to an equation of form (4) over the range 8–100 $\Omega$ is straightforward. The results, using

$$T = 0.835 \exp(-0.62/R_{\text{sheet}})$$

are given in Table 1

### 2.2. Real cell

The equivalent electronic circuit of a real cell shown in Fig. 3 was used to simulate a cell comprising $N$ elemental cells in parallel, supplied with a level of illumination determined by an external sun level modified by a transmittance calculation based on the conductive film transparency (Eq. (7)).

The visible (photopic response) spectrum is used because DSC are only sensitive to visible radiation not IR. Ideally the weighting function should correspond to the dye response.

As explained earlier, the value of the internal resistances used in any particular element depend on scaling the value of a 1 cm$^2$ cell according to the element thickness; a 1 mm $\times$ 1 cm cell would have a total resistance of around 45 $\Omega$, and so on. As the cell resistances scale, so must the saturation currents of the table look up the diode together with the conversion constant inherent in the photocurrent generator. Not so obvious is the fact that the parameter $z$ in the illumination calculator also has to scale, because the circuit computes the emulated illumination

<table>
<thead>
<tr>
<th>Sheet resistance ($\Omega$)</th>
<th>Stated transparency</th>
<th>Fitted transparency</th>
</tr>
</thead>
<tbody>
<tr>
<td>8</td>
<td>0.77</td>
<td>0.773</td>
</tr>
<tr>
<td>15</td>
<td>0.8</td>
<td>0.801</td>
</tr>
<tr>
<td>80</td>
<td>0.83</td>
<td>0.829</td>
</tr>
<tr>
<td>250</td>
<td>0.85</td>
<td>0.833</td>
</tr>
</tbody>
</table>

Because of discrepancies where $R_{\text{sheet}} \approx 250 \Omega$, Eq. (4) is taken to be valid only in the range $8 \Omega < R_{\text{sheet}} < 100 \Omega$. 
level from the absolute value of the sheet resistance used in the model, and not the value referred to a cell of constant area.

3. Results

The IV plot of an elemental cell was checked and compared with appropriately scaled curves from experimental cells. Figures for the series resistances were selected on the basis of most accurate fit to a similar real cell. A series resistance of 4.5 $\Omega$ was required for most accurate simulation, based on a 1 cm$^2$ cell. Actual figures for an elemental cell were scaled from this.

The effect of using this design of elemental cell to emulate a 0.1 cm$^2$ cell is shown in Fig. 4. The scaled short-circuit current is 14 mA cm$^{-2}$, typical of the values observed in real cells at STI. It should be noted that this circuit element makes no attempt to simulate the behaviour of a real element at AC. Electrical impedance spectroscopy of the simulated element would not resemble that of a real cell element.

A complete cell is emulated by forming a transmission line of elemental cells separated by resistances representing sheet resistance of the conductive oxide. The sheet resistances and illumination level at the cells was linked according to Eq. (1). The resulting circuit has been shown in Fig. 3.

In order to determine the most suitable number of elemental cells required to emulate a real cell of given size, a check was performed where a 5 mm real cell was simulated by a varying number (5, 10, 20 and 40) of elemental cells. The fill factor at maximum power point was calculated, and plotted against number of elements used in the simulation. Cells emulated with only five elements deviated substantially from cells with larger number of elements, especially at higher power levels typical of cells being operated under realistic conditions. It was therefore considered that 20 elemental cells would be the minimum necessary to produce reliable results for a real array. The energy output of such an emulated cell would approach its asymptote to closer than 1% at one sun insolation.
Varying the resistivity and hence the transparency of the glass produced a family of curves expressing light output against resistivity, as indicated in Fig. 5. An optimum value of sheet resistance was found under these conditions of approximately $R = 15 \, \Omega/\square$, refer Fig. 5, and at this value the electrical and optical losses will be equal. The simulator may also tend to overstate optical losses because the figures relating optical losses to sheet resistance are stated for air:film interfaces, not electrolyte:film interfaces. The latter will recover slightly lower losses due to the closer refractive indices of the film and liquid.

Other workers have recognised that maximising the performance of cells depends achieving an optimum conducting film thickness, but have tended to the view that the optimum is independent of cell size [16]. To check this, the above simulation was run using 2 cm long cells, being simply two 20 element strings in series. The results of this experiment clearly indicated that the optimum resistivity for the TCE does depend on cell size, and indeed, that real cells have a definite upper limit to useful length. In the example chosen, the optimum TCE resistance for the 2 cm long cell is $7 \, \Omega/\square$ compared to $15 \, \Omega/\square$ for the 1 cm long cell, but the maximum power output is only 52% greater than for the 1 cm long cell, although it occupied twice the useful area. This is again in accordance with expectations because the optical losses of both cells will be the same, so in order to produce the same electrical loss with a cell of increased length, the sheet resistance must decrease.

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**Fig. 4.** $I/V$ Plot of a 1 mm long DSC elemental circuit over the range 0–1 sun.
The substantial interaction effects, now evident, between the sun level and sheet resistance strongly suggested the need for a more detailed investigation of their combined effects on efficiency at maximum power point (mpp), and hence for a similar manufacturing cost, on the cost of electricity generated. A simulation of a 1 cm × 1 cm cell was run to find the peak efficiencies when the cell was constructed using conductive sheet resistances from 8 to 48 Ω/sq and at 0.1 suns, 0.3162 suns and 1.0 sun. The results are given in Fig. 6.

Note the strong interaction between the sun level and the sheet resistance. The cell gives significantly poorer performance at high sun, with the efficiency reaching 74.2% of that obtained at a different sheet resistance at low sun. For a cell optimised at low sun, the highest relative efficiency that could be expected at high sun would be only about 55% of that obtained under the conditions for which the cell had been optimised.

In order to compare once again the effect of varying the electrical length of the cell, the simulation was repeated using a 2 cm long, 2 cm² cell. The results indicated that all the peak power points are reached at about half the sheet resistance required for the 1 cm² cell.
It is clear that for cells operated in BIPV systems, where the incident solar radiation is rarely if ever near 1 sun at normal incidence, substantially better performances would be obtained using sheet resistances in the region of $25 \, \Omega/\square$ with corresponding higher transparency. It is clear that the transparency of the film is of greater concern than its resistivity.

The effect on the cost of generated electricity can be significant. As will be shown later, the total energy delivered over, say, a year, depends on the relative insolation levels experienced by the cell. A histogram of intensities versus time can be used to determine which level of light the cell should be optimised for.

4. Experiment

In order to verify the ability of the simulator to model real cells in modules of various sizes, two commercial modules, one containing four cells in series and one...
containing six cells in series, were characterised using a conventional solar simulator and an IV characterization system.

The modules were constructed at STIs manufacturing facility using standard production techniques, similar to those generally available publicly. Each module, or tile comprises a number of single cells laid end to end, with the current path from one side of the tile to the other, through the cells in series. Cell interconnects were made from metal loaded polymer, which also provided inter-cell sealing and so removed potential pathways for short-circuit currents to flow.

Experimental module characteristics are given in Table 2. The cell electrical length is annotated as ‘width’ in the diagram, and cell electrical width annotated as ‘length’. This follows from conventional references to objects with high aspect ratios, but the term length (electrical length) in the context of the simulation refers to the path length along the current flow. Interconnect gaps refer to the distance between the individual cells on the tile. The external connection gap refers to the external distance from one of the outer cells to the current collection finger. The total external resistance is the sum of the resistances of the interconnect gaps and the external connections.

The values of salient parameters in the cell simulator (sheet resistance, element series resistance, recombination saturation current, and photo-determined shunt resistance) were adjusted to produce the best possible fit. Each tile could be simulated individually to an accuracy of about ±0.5%, although because the tiles were not matched, the simulator parameters were not the same. Optimising the fit for one tile, and then entering identical parameter values for the other tile tended to give about a 10% error in the curves for the second tile in the worst case. The results are shown in Fig. 7.

5. Discussion

It has shown here that it is possible to use electronic circuit analysis tools to simulate an electrochemical system with good accuracy. Circuit simulators are rarely called upon to model devices with attributes not easily expressed by combinations of conventional circuit elements such as resistors and diodes. The simulation of a DSC element using a circuit simulator with function generators, and the extension of this

<table>
<thead>
<tr>
<th>Parameter</th>
<th>4-cell module</th>
<th>6-cell module</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cell length (along current flow) (mm)</td>
<td>19.5</td>
<td>12</td>
</tr>
<tr>
<td>Cell width (transverse to current flow) (mm)</td>
<td>168</td>
<td>166</td>
</tr>
<tr>
<td>Interconnect gaps (mm)</td>
<td>3</td>
<td>5</td>
</tr>
<tr>
<td>Gap width (mm)</td>
<td>3</td>
<td>3</td>
</tr>
<tr>
<td>External connection gap (mm)</td>
<td>4</td>
<td>4</td>
</tr>
<tr>
<td>Total external resistance (whole module) (Ω)</td>
<td>1.52</td>
<td>2.08</td>
</tr>
</tbody>
</table>
The process to model an entire tile of 6 cells each typically of 24 circuit elements of 0.5 mm length along the current flow, is a significant step on the way to be able to predict the behaviour of entire solar arrays from first principles.

The results demonstrate that it is possible to develop a useful DSC emulator, incorporating a number of features specific to these types of cells. The simulation has produced results expected from earlier work, and also novel results. Future work will include checking these results with other combinations of parameters accurately adjusted to those of production cells.

Cell and tile simulation can yield accuracies of current at a given voltage of the order of ±0.5% of short-circuit current for tiles of six individual cells. Future refinement should improve this, and permit accurate investigation of lesser order effects such as those arising from shunt impedances.

The design of a cell simulator for individual cells is not entirely the whole solution to the construction of highly cost-effective DSC arrays. There are other structures
which tend to take up assembly area and do not contribute directly to cell output, such as seals, guard spaces and interconnects from one side of the assembly to the other. In computing the performance of an assembly of DSCs in a panel it must be borne in mind that the goal is to build a device which generates electrical energy for the least cost, not one that necessarily converts some level of insolation into the highest possible power. Because sunlight is essentially free, these are not at all the same thing. The production processes which determine both the array efficiency and the array cost will invariably contain many parameters. It has been indicated earlier that there is little or no marginal cost associated with selecting one set of parameters over another.

Firstly, a general cost minimum has to be sought, balancing the production process complexity against the cell performance, as indicated in Fig. 8. A clear minimum for the ratio

\[
\frac{\text{process cost}}{\text{cell efficiency}}
\]

is invariably found.

Below some level of process complexity, the cells will not work at all, so the efficiency is effectively zero. As the processing becomes more complex, the efficiency rises, but tends to an asymptote determined by the physical properties of the technology. Process costs however rise fairly linearly with complexity all the while. The cost of generated electricity is closely determined by the parameter of process cost divided by cell efficiency, so falls from infinity to a hopefully low value, then rises as technology limitations start to dominate.

Having selected a level of process complexity commensurate with achieving a reasonable cost of electricity minimum, this paper now shows that further improvement can be made at little or no marginal cost by adjusting production process parameters, as indicated in Fig. 9. This is the value which the plant process control system has to attempt to maintain.

![Fig. 8. Indicative chart relating the effect of varying manufacturing process complexity on cost of electricity generated by a solar array.](image-url)
This paper has shown ways in which DSSC’s can be designed to operate close to the minimum as indicated in Fig. 9 above. Further work will refine this and introduce the effect of considering and varying other attributes of the arrays to approach even more closely the minimum cost of electricity possible for the array.

Acknowledgements

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References


