1. Methodology

**2.1) I-V data importer**

To fulfil the goal of high throughput characterization, a MATLAB routine that imports I-V data to the workspace was paramount. The VMP3 16 -channel potentiostat in the research labs of ACEX will export raw I-V data in text (TXT) files, and therefore this program was designed to read only TXT file. The program expects the TXT file to contain voltage and current data in the first and second column respectively with no headers; the current and voltage data were then stored temporarily in single column arrays and used for subsequent analysis.

In standard MATLAB coding practice, the main file, function files and other data to be imported are all grouped in the same folder. However, the program is expected to be used for datasets by multiple researchers, and therefore a likelihood that some important function files may be deleted in the process of removing old TXT files to accommodate new ones exists. Hence, separate folders were made for the function files and the data files; the folders must be labelled as ‘Funcfiles’ and ‘Datafiles’ otherwise the program will return an error.

**2.3) Extracting Isc and Voc**

To extract accurate and values, the current data is first smoothed using the *“rlowess”* smoothing function in MATLAB. This function fits a first order polynomial and minimizes the weighted least squares for a small set of data and rejects data six mean absolute deviations [1][2].

The program assumes the datafiles contain I-V data for the two non-active quadrants because interpolation was used to calculate Isc and Voc. The nearest two current datapoints in first and second quadrants were interpolated to obtain Isc, and similarly the nearest two voltage datapoints in the second and third quadrant to obtain Voc.

**2.4) Extracting and**

The extraction of Vm and Im will be affected by the direction of the scan as arrays are. In the forward scanned data Im and Vm will have a higher index in array where this is the opposite in reversed scaned data. The program can identify if the data scan direction by comparing the index positions of Isc and Voc in the current and voltage column vector. The dot product on the current and voltage vector is carried out to obtain a power vector. The program seeks the maximum power in this vector and returns the Vm and Im which produced the maximum power.

**2.5) The gradients of the curve that x and y intercept**

**2.6) Simulated I-V data generation for fixed Voc and Isc**

To determine the accuracy of the estimated parameters, simulated data with known parameters were fitted. The single diode model photovoltaic model, which is implicit in nature, can be expressed as an explicit form using the lambert W function.

The program is expected to be robust for many different types of I-V curves, but currently it is expected that most I-V curves that will be tested will be for perovskite solar cells. Good perovskite solar cells have a fill factor [] and with an Isc and Voc of 20 mA/cm^2 and 1V. Data was simulated for a 1 pervoskite solar cell that produces an Isc of 20mA and a Voc of 1V for different parameters. For this report a 8 combinations of parameters were used to generate the simulated data, which are shown in the table below.

|  |  |  |  |
| --- | --- | --- | --- |
| **Case** | **Rs** | **Rsh** | **n** |
| 1 (low Rs, High Rsh, low n) |  |  | 1 |
| 2(high Rs, High Rsh, low n) |  |  | 1 |
| 3(low Rs, Low Rsh, low n) |  |  | 1 |
| 4(low Rs, High Rsh, high n) |  |  | 5 |
| 5(high Rs, Low Rsh, high n) |  |  | 5 |

Table : The table summarises the parameters used to generate eight I-V simulated data for Isc = 20mA and Voc = 1 V.

These parameters were chosen because of the shape of the I-V plot differs greatly, and the algorithm is expected to fit the data robustly.

**2.7) Initial parameter guessing methods**

In numerical methods the initial guesses are very important and they must be close to the actual solution to converge 1. In this study three analytical methods were considered to obtain initial guesses.

1. **Phang’s method**

Phang’s method provides an analytical solution to all the 5 device parameters if and are known2. Since these parameters are known, the following equations can be solved to find initial guesses for and .

1. **Zhang’s method modified**

Zhang’s approach to obtaining initial guesses was through the fitting of experimental data points to the equation given below, which has the form of a straight line.

The gradient was calculated for 6 points and then equation 4 was fitting, but their method of choosing the data points were not explained. Hence, we attempted solve the equation at the and where data is readily available.

Equation 6 and 5 can be subtracted to obtain to as function of known parameters.

can be retrieved by substituting the calculated in into equation (5). Equation (5) has been rearranged below to make as the subject of the formula.

**2.8)**

**2.9) Nonlinear least squares fitting**

The MATLAB provides two algorithms which changes the parameters it has been supplied with to minimize the least squares between the fitted curve and the experimental data. The levenberg-marquardt most commonly used algorithm. However, this method cannot be constraint and negative parameters are possible if the starting guesses are not near the actual solution. There the trust region method was implemented as containsts are permitted in this algorithm. The lower bound is maintained as

An initial guess vector was created in MATLAB which contained the . The value was maintained as , but the value was calculated from the Zhang method and the value from the Phang method. The algorithm was set as trust region reflective and the tolerance step size and was set as and the function tolerance was set as with the maximum number of iterations set to 1000.