A new approach to transfer characteristic slope estimation

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ABSTRACT

Organic field-effect transistors (OFETs) have found a wide range of uses due to their attractive properties. A great deal of effort has been expended on boosting their mobilities, which tend to be low. Given this, accurate estimation of the mobility is crucial. We have developed a web application that automates or simplifies several of the steps required to estimate the mobility from experimental data. The app can be accessed at `ofetanalysisapp.shinyapps.io/ofetanalysisapp`. The app takes as inputs a file with the data and pieces of information like the number of OFETs and their channel lengths. The app has features that enable the user to mark OFETs as outliers, which are excluded from subsequent calculations. It fits nonlinear regression models to compute estimates of the mobility as well as the threshold voltage. The app provides several visualizations that give the user insight into the nature of the data. The estimates computed by the app can be downloaded in an Excel file so the user can perform further analysis. The use of the app is illustrated with a dataset from one of our OFET experiments.

Keywords: Mobility, estimation, statistics

1. INTRODUCTION

Organic field-effect transistors (OFETs) are becoming more popular because of their ability to complement traditional silicon technology. They are used in a variety of applications, such as artificial skin, RFID tags, flexible devices,[1] and biological sensors.[2] There are several reasons for their versatility. They can be made from a number of different materials, be grown on flexible substrates, and be processed at low temperatures. They weigh little and are biodegradable. However, compared to field-effect transistors (FETs) that are silicon-based or inorganic, these devices have some drawbacks, like low mobilities and slow processing speeds.

Much work has been done to increase their mobilities over the last decade.[3] The mobility is estimated with a plot of the square root of the drain current versus the gate voltage. A straight line is fit in the saturation regime, and its slope is used to calculate a mobility estimate. This estimate is quite sensitive to changes in the measured value of the slope.[4] An improper fit often results in an overestimate.[5,6] Accuracy can be improved by making the fit better. It can also be improved by combining estimates from many OFETs. Highly automated systems for measurement, data processing, and estimation are essential for this approach, as many measurements need to be made and a large amount of data must be wrangled. To carry out this approach, we have been using a measurement system called MBox and a web application for data processing and estimation that we have developed.

We illustrate the use of the MBox system and the app with data from experiments on optimizing the quality of the dielectric layer of an OFET. The quality of that layer plays a crucial role in the performance of an OFET. Several methods are used to prepare this layer in practice. We have employed a simple and cost-effective method, anodization, to grow high-quality aluminum oxide on the aluminum gate. Optimization was done with respect to the amount of anodization current and the duration of the current. The optimization experiments are described in Sec. 2. Section 3 shows how the app can be used to process data from an experiment and compute estimates. Results from the experiments are presented in Sec. 4.

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2. EXPERIMENTAL DETAILS AND DEVICE CHARACTERIZATION

An OFET is similar to a standard FET. A schematic diagram of an OFET is shown in Fig. 1. Each 21.5 mm by 21.5 mm square glass substrate was cleaned according to a standard protocol: ultrasonic cleaning in soapy water followed by cleaning with acetone, methanol, and isopropyl alcohol. OFETs were then grown on each substrate according to the following procedure. First, a 150-nm-thick structured aluminum film was laid on the substrate by thermal deposition. This film served as the gate through which an electric field was applied to the transistor.

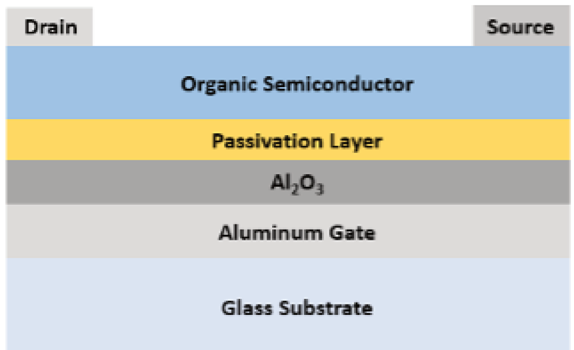

Figure 1. A schematic diagram of an OFET.

Following Majewski et al. (Ref. 7), a standard anodization process was used to grow on the aluminum film a 10-nm-thick aluminum oxide dielectric. A 1-mM citric acid solution was prepared by dissolving citric acid crystals in DI water. In the solution were placed a platinum electrode, which served as a cathode, and the glass substrate topped with an aluminum film, which served as an anode. Electrolysis was then carried out by supplying constant current through the circuit. A schematic of this process is shown in Fig. 2.

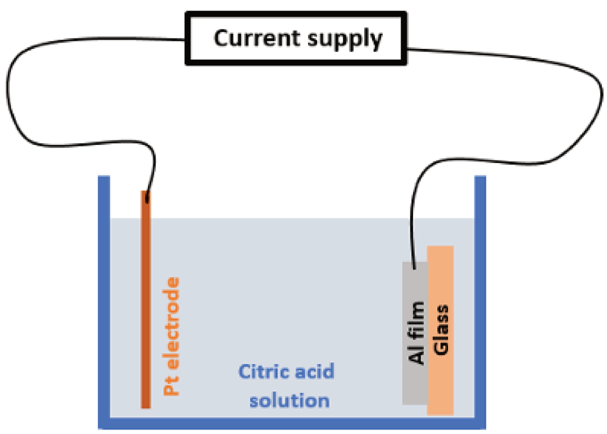

Figure 2. A schematic of the anodization process carried out on the aluminum film deposited on the glass substrate.

The passivation layer was a Tetradecylphosphonic acid (TDPA) self-assembled monolayer (SAM); it was created by immersing, for 18 hours, the substrate and previously created layers in a 5-mM TDPA solution that was prepared with isopropyl alcohol. Next, a 60-nm-thick C_{60} organic semiconductor film was formed above the passivation layer by thermal deposition. Finally, the 20-nm-thick aluminum source and drain were placed on top using a structured shadow mask.

Depending on the nature of the semiconducting material, and with the application of suitable potential through the gate electrode, a proper channel could be formed on the semiconductor film. A flow of current could be established through it from the source to the drain. Hence, the flow of current through the device could be controlled by a suitable application of the voltage at the gate, and the transistor could be turned on or off.

Figure 3 shows C_{60} OFETs grown on a single glass substrate; the OFETs are the squares in the center. The 12 OFETs have six different channel lengths.

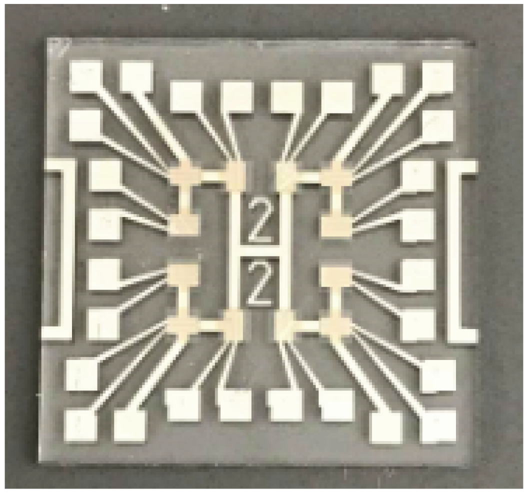

Figure 3. C_{60} OFETs grown on a single glass substrate. The 12 OFETs are in the center and have six different channel lengths.

The growth and quality of the aluminum oxide strongly depend on the amount and duration of the anodization current. A detailed study of the effect of these two factors was carried out according to the experimental plan shown in Fig. 4. In this experiment, 16 substrates, each containing 12 transistors, were processed. Each substrate was processed with an anodization current between 0.2 mA and 0.5 mA and an anodization time between 200 sec and 800 sec. A different pair of current and time was used for each substrate. The effect of these two variables on the performance of the devices was studied using the transfer characteristics of the devices. An automated measurement system, Mbox, shown in Fig. 5, and the Keithley 4200 semiconductor characterization system were used to characterize the OFETs. A dual gate sweep from -1 V to 3 V was applied to study the transfer characteristics of the devices, with the drain kept at 3 V.

		Anode Current (mA)			
		0.2	0.3	0.4	0.5
Anodization Time (Sec)	800	00	01	02	03
	600	10	11	12	13
	400	20	21	22	23
	200	30	31	32	33

Figure 4. Experimental plan for the anodization condition variation. Anodization time and current were varied. Each square represents a substrate; the numbers displayed are the substrate numbers.

The performance of the OFETs was quantified by estimating the mobility, the threshold voltage, and the hysteresis from the transfer characteristic data. We have developed a web application located at ofetanalysisapp.shinyapps.io/ofetanalysisapp that can process experimental data and estimate these parameters. In the development of the app, our goals have been to automate as much of the data analysis as possible, to reduce subjectivity in the analysis, and to enhance reproduciblity. The app was created using the shiny package of the programming language R; see Ref. 8 for information on shiny. Section 3 illustrates the use of the app with data from the anodization experiment in which the current was 0.5 mA.

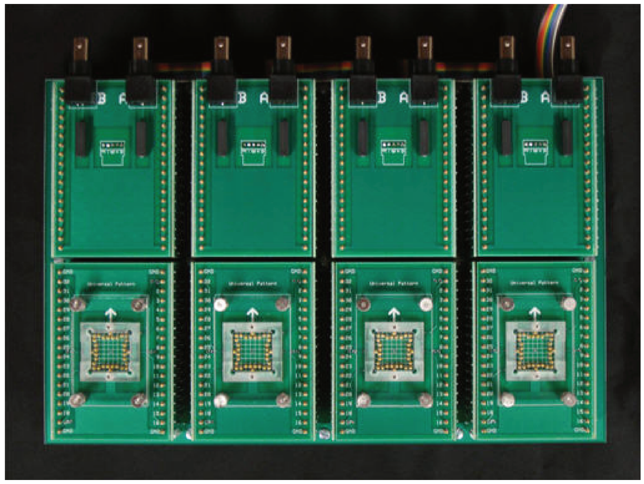

Figure 5. An automated measurement system, MBox, used in the characterization of the OFETs. With this system, 48 transistors can be characterized at a time.

3. USING THE APP

The app is divided into several tabs. The Directions tab has directions for using the app and links to videos that show how to use it. The next few sections describe the most important of the other tabs.

3.1 The Main Tab

The user must begin on the Main tab, which is shown in Fig. 6. The user selects a file to upload at the top. The file must be an Excel file with one sheet for each OFET in the experiment. A sheet for an OFET is expected to have a column giving the gate voltages that were swept over and a column giving the saturation drain current measured at each gate voltage. The dropdown lists at the top of the Main tab allow the user to specify the names of the gate voltage and drain current columns.

Next, the user indicates whether the OFETs in the experiment were n-type or p-type and enters the number of OFETs the experiment involved. It is assumed that the OFETs' channel lengths formed a periodic sequence. For the file in Fig. 6, the channel lengths of the first six OFETs were 200, 150, 300, 350, 100, and 250 µm, as were the channel lengths of the next six OFETs, etc. The repeating portion of the sequence goes in the channel length pattern box. Another assumption is that the OFETs had the same channel width and the same gate capacitance. These go in the next two boxes.

The app computes parameter estimates for each OFET and for each group of OFETs. The user can either choose to group the OFETs by sample or by channel length. If the user chooses to group the OFETs by sample, then they must also enter a sample size. For example, in Fig. 6, the user has decided to group by sample and the sample size is 12. The first group will consist of the first 12 OFETs, the second group will consist of the next 12, etc. Thus, for the anodization data, each group corresponds to a particular anodization time - the first group corresponds to a time of 800 sec, the second to 600 sec, the third to 400 sec, and the fourth to 200 sec. If the user instead groups by channel length, then each group will consist of all the OFETs with a particular channel length.

Finally, the user must decide whether to compute parameter estimates using the OFETs' forward sweeps or their backward sweeps.

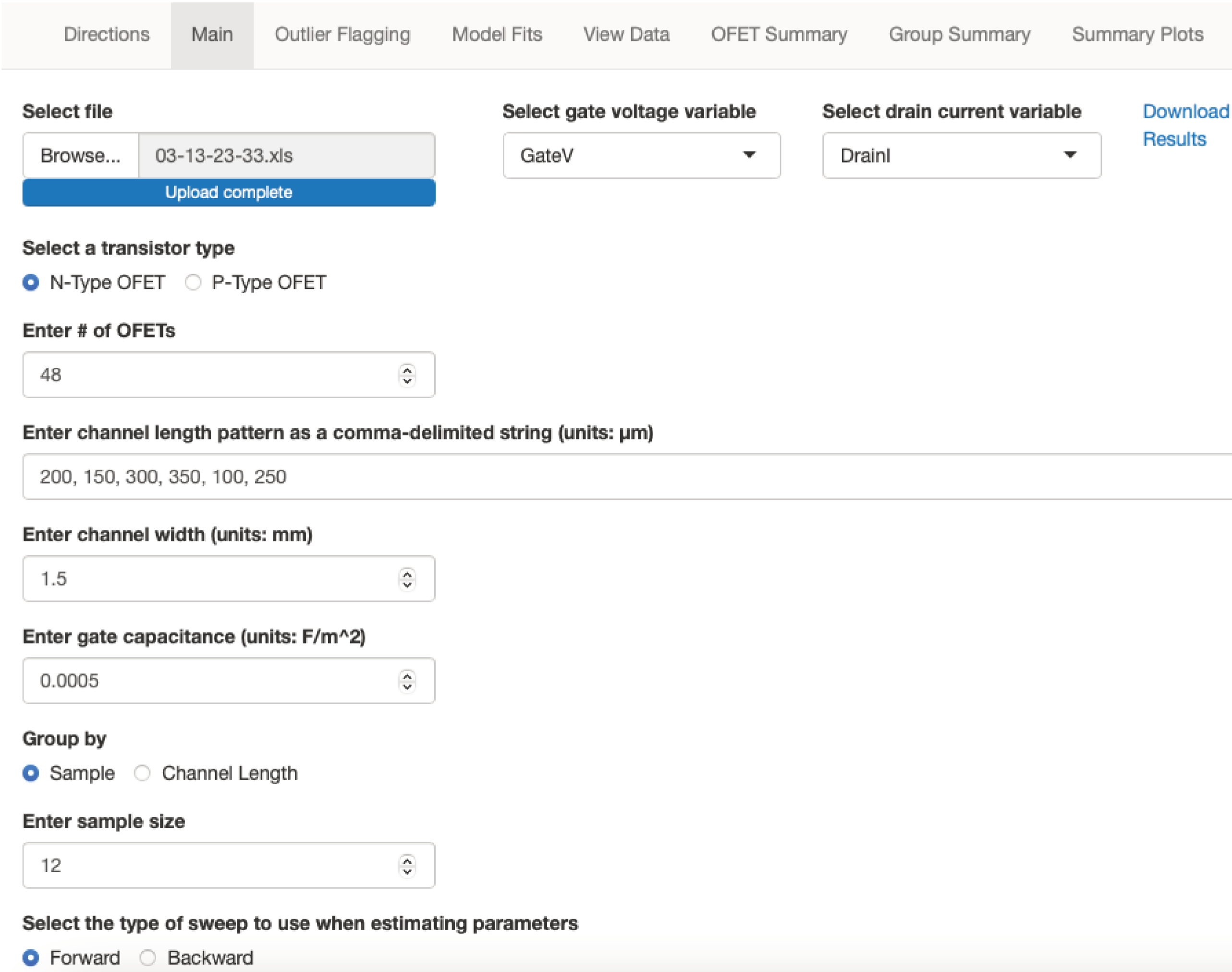

Figure 6. The Main tab of the app.

3.2 The Outlier Flagging Tab

Once the user has finished with the Main tab, they can move on to the Outlier Flagging tab, where they can flag OFETs as outliers if the data for them looks abnormal. This is an important step, as using parameter estimates for outlier OFETs to compute group-level parameter estimates can yield inaccurate numbers. OFETs flagged as outliers are excluded from the calculations of the group-level estimates.

The Outlier Flagging tab is shown in Fig. 7. In the plot, the square root of the drain current is plotted against the gate voltage for each OFET. The curve for each OFET consists of the OFET's forward and backward sweeps. As shown in Fig. 7, if the user puts their cursor over a curve, then the number of the corresponding OFET will be displayed. If they click on that number in the dropdown list, then the OFET will be flagged as an outlier if it previously wasn't being flagged, or unflagged if it previously was being flagged. This change is shown in Fig. 8.

If the user clicks on the button labeled "Use suggestions", then the app will run an outlier detection algorithm and flag only the OFETs it classified as outliers. If the data is very messy, then the algorithm may fail to identify any outliers. If this happens, then the app will display a message saying that no suggestions can be made.

If the data is not too messy, then the user may be able to spot all of the outliers in the plot on this tab. Otherwise, they may have to look at the OFETs one-by-one to spot the outliers. This and other tasks can be done on the next tab, the Model Fits tab.

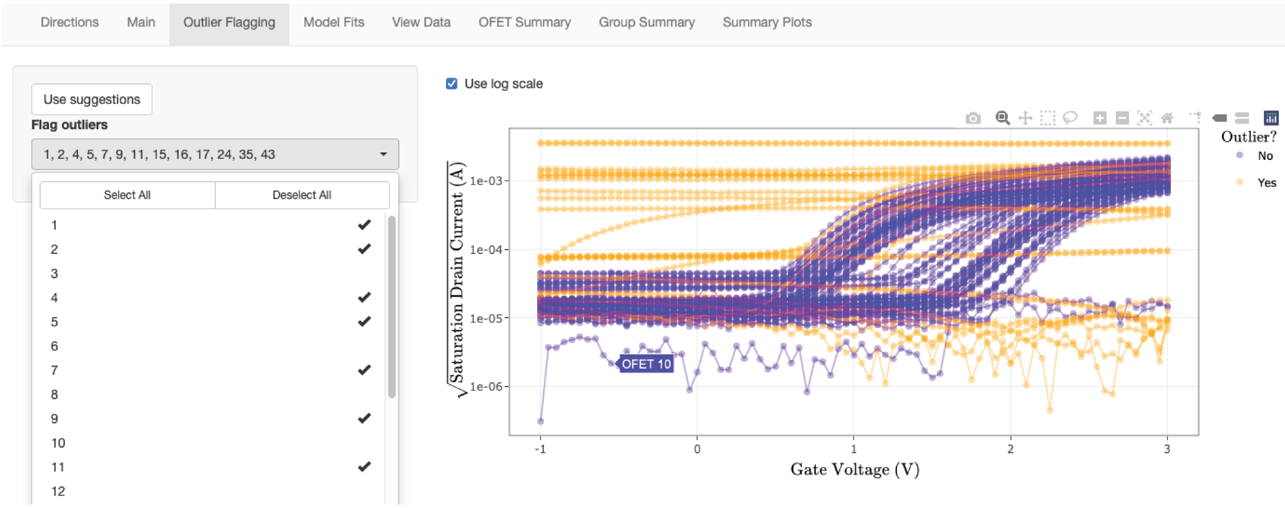

Figure 7. On the Outlier Flagging tab, putting one's cursor over the curve for an OFET causes the OFET's number to be displayed.

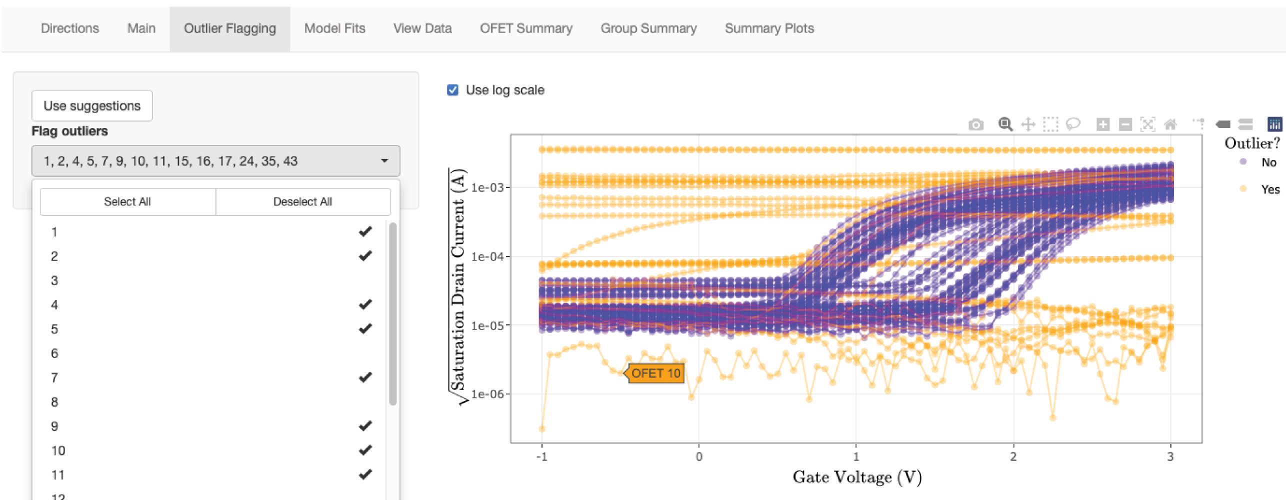

Figure 8. On the Outlier Flagging tab, clicking on an OFET's number in the dropdown list causes it to be flagged or unflagged.

3.3 The Model Fits Tab

The Model Fits tab is displayed in Fig. 9. On this tab, for the OFET entered in the box at the top, the plot on the left displays the nonlinear regression model fit to the forward sweep and the nonlinear regression model fit to the backward sweep. Both models are of the form

$$\sqrt{I} = \max\{\gamma, \alpha + \beta V\} + \epsilon, \tag{1}$$

where I represents the drain current, V represents the gate voltage, and ϵ is a random error term. As the figure shows, a fitted model of this form has a flat piece and a slanted piece. Let $\hat{\gamma}$, $\hat{\alpha}$, and $\hat{\beta}$ be the estimates of γ, α, and β, respectively. Then the flat piece has intercept $\hat{\gamma}$; the slanted piece has intercept $\hat{\alpha}$ and slope $\hat{\beta}$. The threshold voltage can be estimated as the gate voltage at which the slanted piece intersects the gate voltage axis, or

$$-\frac{\hat{\alpha}}{\hat{\beta}}. \tag{2}$$

The mobility can be estimated as

$$\frac{2l\hat{\beta}^2}{wc_g}, \tag{3}$$

where l, w, and c_g are the channel length, channel width, and gate capacitance, respectively. Note that this approach does not require the researcher to choose a gate voltage range over which to perform linear regression. Such a choice is subjective and could lead to an unjustifiably high mobility estimate. It could also makes the results harder to reproduce, as one might have to guess which range was used in order to reproduce them.

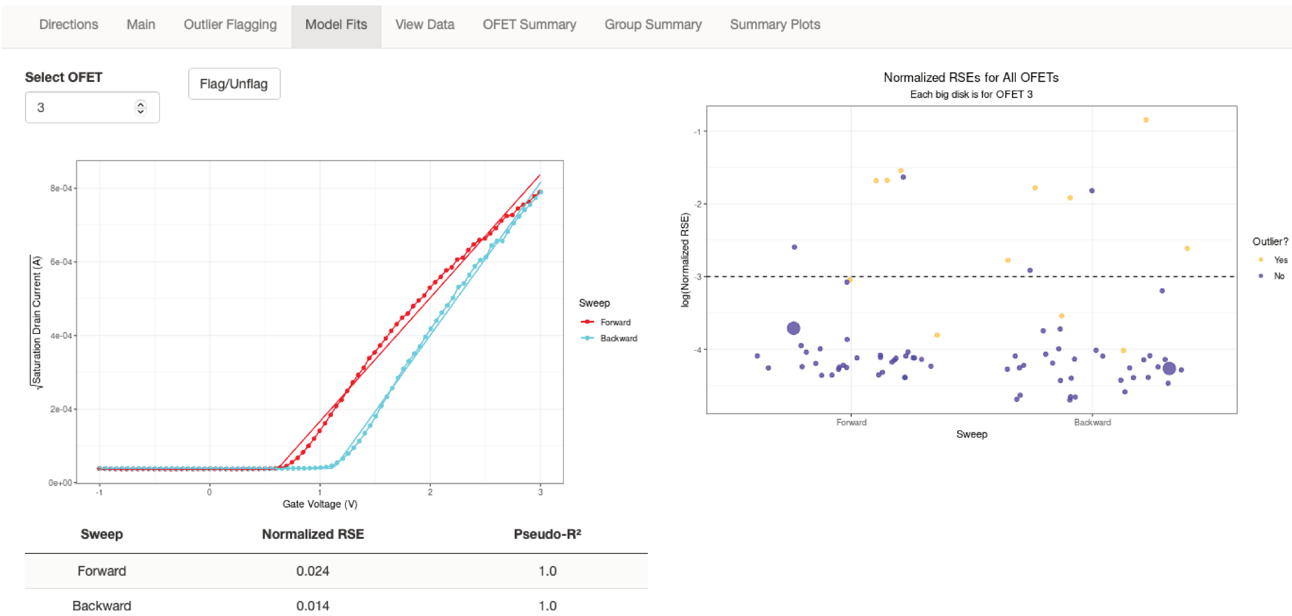

Figure 9. The Model Fits tab.

The fit for one sweep might be better than the fit for the other. The plot enables the user to compare the fits visually. The fits can also be compared using the two measures of quality of fit, the normalized RSE and the pseudo-R^2, in the table below the plot. The RSE can be viewed as the average deviation of a sweep from the model fit to it. This average is normalized by dividing it by the square root of the drain current at the largest gate voltage. Normalization makes it possible to compare different sweeps, which could have different drain current ranges. The pseudo-R^2 can be interpreted as the proportion of variance in the square root of the drain current explained by the gate voltage. The closer this is to one, the better the model fits.

The plot on the right shows the logarithm of the normalized RSE for every sweep of every OFET. The dashed line is at -3; in our experience, outlier OFETs tend to lie above -3 and inlier OFETs tend to lie below it. If the set of points for one sweep type is considerably higher than the set of points for the other sweep type, then the forward and backward sweeps must look quite different. Something may have gone wrong during the experiment; it might not be a good idea to proceed with the analysis. In the figure, the two point sets are similarly positioned. The user could choose to compute parameter estimates using the backward sweeps since their normalized RSE values are somewhat smaller. To do this, the user would have to return to the Main tab and select "Backward" at the bottom (see Fig. 6).

If the user looks at the plot on the left and changes their mind about the inlier/outlier status of an OFET, then they can click on the "Flag/Unflag" button at the top to change the status.

3.4 The Summary Tabs

The OFET Summary tab shows a table with one row for each OFET; see Fig. 10. It summarizes at the OFET level the information the user has entered, like outlier statuses and channel lengths, and displays parameter estimates. The "Was Model Fit?" column shows whether the nonlinear regression model was fit to the indicated sweep; it will show "No" if the sweep looks very different from the model.

Figure 11 is a screenshot of the Group Summary tab. For each group, it shows the number of inlier OFETs and outlier OFETs. The parameter estimate for each group is computed from the parameter estimates for the inlier OFETs in it. For example, the threshold voltage estimate for group 0 is the average of the threshold voltage estimates for the inlier OFETs in group 0. The error for a parameter estimate is a measure of the uncertainty in the estimate. For example, the group 0 threshold voltage error is the standard error of the mean of the threshold voltage estimates for the group 0 inliers. For a set of values, the standard error of the mean is the standard deviation divided by the square root of the number of values. It measures the uncertainty in the mean of the values.

Directions | Main | Outlier Flagging | Model Fits | View Data | OFET Summary | Group Summary | Summary Plots

Show 10 entries

Group	Grouped By	OFET	Outlier?	Channel Length (μm)	Channel Width (mm)	Gate Capacitance (F / m²)	Sweep Used	Was Model Fit?	Threshold Voltage Estimate (V)	Mobility Estimate (m² / (V · s))	Hysteresis (1 / V)
0	Sample	1	Yes	200	1.5	0.0005	Backward	No			0.0000038
0	Sample	2	Yes	150	1.5	0.0005	Backward	No			0.0000070
0	Sample	3	No	300	1.5	0.0005	Backward	Yes	1.0	0.00014	0.00022
0	Sample	4	Yes	350	1.5	0.0005	Backward	Yes	0.81	0.00071	0.00033
0	Sample	5	Yes	100	1.5	0.0005	Backward	Yes	-4.8	0.000013	0.00066
0	Sample	6	No	250	1.5	0.0005	Backward	Yes	1.2	0.00075	0.00086
0	Sample	7	Yes	200	1.5	0.0005	Backward	Yes	-0.31	0.00012	0.00049
0	Sample	8	No	150	1.5	0.0005	Backward	Yes	0.26	0.000037	0.00019
0	Sample	9	Yes	300	1.5	0.0005	Backward	Yes	-0.51	0.00013	0.00062
0	Sample	10	Yes	350	1.5	0.0005	Backward	Yes	0.37	6.1e-8	0.000045

Showing 1 to 10 of 48 entries — Previous 1 2 3 4 5 Next

Figure 10. The OFET Summary tab.

Directions | Main | Outlier Flagging | Model Fits | View Data | OFET Summary | Group Summary | Summary Plots

Group	Grouped By	Number of Inliers	Number of Outliers	Threshold Voltage Estimate (V)	Threshold Voltage Error (V)	Mobility Estimate (m² / (V · s))	Mobility Error (m² / (V · s))	Hysteresis (1 / V)	Hysteresis Error (1 / V)
0	Sample	4	8	1.1	0.33	0.00046	0.00022	0.00051	0.00018
1	Sample	8	4	1.8	0.039	0.00087	0.00021	0.00085	0.000075
2	Sample	11	1	1.8	0.034	0.00083	0.00019	0.00080	0.000060
3	Sample	11	1	2.0	0.036	0.00070	0.00017	0.00062	0.000072

Figure 11. The Group Summary tab.

3.5 The Summary Plots Tab

The Summary Plots tab has three plots, each corresponding to one of the threshold voltage, the mobility, and the hysteresis. Figure 12 is a screenshot of this tab. In each plot, there is one boxplot for each group. As mentioned previously, groups 0, 1, 2, and 3 correspond to anodization times of 800, 600, 400, and 200 sec, respectively. Parameter estimates that are for outlier OFETs or are very small or very large are excluded. We see that the threshold voltage when the anodization time is 800 sec tends to be smaller than it is for the other times. We also see that there is little difference in mobility across times, though there seems to be greater variation in mobility when the anodization time is 800 sec.

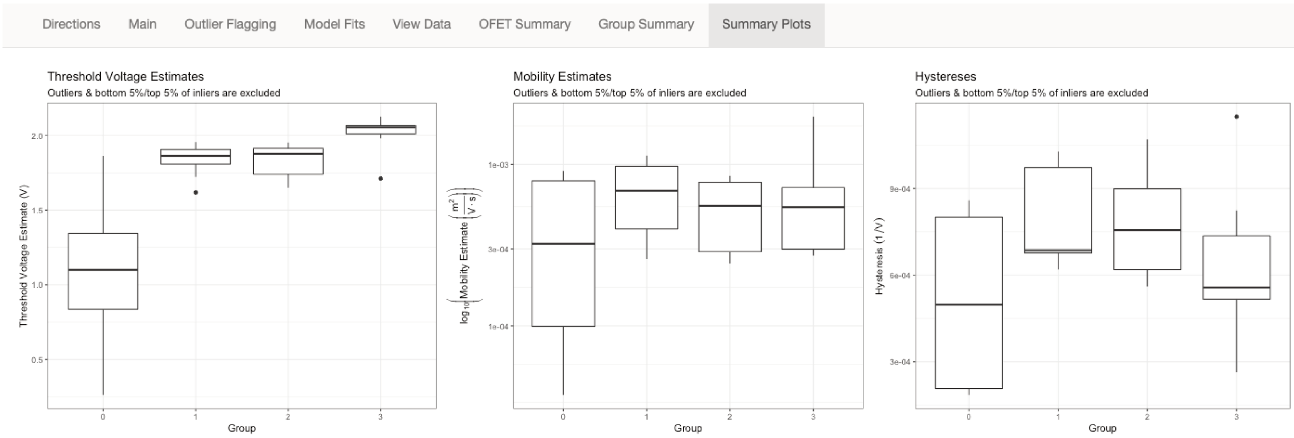

Figure 12. The Summary Plots Tab.

3.6 The Main Tab - Downloading the Results

The results can be downloaded by clicking on a link at the top of the Main tab (see Fig. 6). What the user gets is an Excel file with three sheets. On the Sweep Summary sheet (Fig. 13), there is one row for each pair of OFET and sweep. The parameter estimates are given as well as the estimates of the nonlinear regression model coefficients. The OFET Summary sheet (Fig. 14) has one row for each OFET. It displays the estimates for the sweeps the user has selected. Finally, the Group Summary sheet (Fig. 15) has one row for each group. It displays the same information as the Group Summary tab (Fig. 11). With the information in this file, the user can perform further analysis.

	A	B	C	D	E	F	G	H	I	J	K	L	M	N
1	OFET	Sweep	Channel Length (m)	Channel Width (m)	Gate Capacitance (F / m²)	Was Model Fit?	Gamma Estimate (√A)	Alpha Estimate (√A)	Beta Estimate (√A / V)	Normalized RSE	Pseudo-R²	Threshold Voltage Estimate (V)	Mobility Estimate (m² / (V · s))	Hysteresis Contribution (1 / V)
2	1	forward	0.0002	0.0015	0.0005	FALSE								4.4356E-05
3	1	backward	0.0002	0.0015	0.0005	FALSE								4.05594E-05
4	2	forward	0.00015	0.0015	0.0005	TRUE	1.4871E-05	2.6504E-05	3.4103E-06	-4.1893699	-6.762434	-7.771922917	4.65194E-09	6.17986E-05
5	2	backward	0.00015	0.0015	0.0005	FALSE								5.47899E-05
6	3	forward	0.0003	0.0015	0.0005	TRUE	3.7469E-05	-0.00016962	0.00033531	0.0244809	0.995457	0.505858513	8.99457E-05	0.001102689
7	3	backward	0.0003	0.0015	0.0005	TRUE	3.888E-05	-0.000426	0.00041451	0.0140744	0.998319	1.027733239	0.000137452	0.000887683
8	4	forward	0.00035	0.0015	0.0005	TRUE	8.2073E-05	-0.0004018	0.00078404	0.0223278	0.996227	0.512476287	0.000573732	0.00255715
9	4	backward	0.00035	0.0015	0.0005	TRUE	8.1764E-05	-0.00070842	0.00086943	0.0180156	0.997405	0.814811232	0.000705521	0.002230421
10	5	forward	0.0001	0.0015	0.0005	TRUE	0.00142929	0.0013626	0.00011115	0.1859293	0.873021	-12.25910978	3.2945E-06	0.006037334
11	5	backward	0.0001	0.0015	0.0005	TRUE	0.00119814	0.00104519	0.00021999	0.0622787	0.972083	-4.751159409	1.2905E-05	0.005377994
12	6	forward	0.00025	0.0015	0.0005	TRUE	1.6866E-05	-0.00029442	0.00077244	0.0746675	0.969807	0.381153028	0.000397781	0.002681843
13	6	backward	0.00025	0.0015	0.0005	TRUE	1.6553E-05	-0.00124653	0.00106397	0.0542706	0.981092	1.171585964	0.000754686	0.001822471

Figure 13. The Sweep Summary sheet.

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q
1	Group	Grouped By	OFET	Outlier?	Channel Length (m)	Channel Width (m)	Gate Capacitance (F / m²)	Sweep Used	Was Model Fit?	Gamma Estimate (√A)	Alpha Estimate (√A)	Beta Estimate (√A / V)	Normalized RSE	Pseudo-R²	Threshold Voltage Estimate (V)	Mobility Estimate (m² / (V · s))	Hysteresis (1 / V)
2	0	sample	1	TRUE	0.0002	0.0015	0.0005	backward	FALSE								3.8E-06
3	0	sample	2	TRUE	0.00015	0.0015	0.0005	backward	FALSE								7.01E-06
4	0	sample	3	FALSE	0.0003	0.0015	0.0005	backward	TRUE	3.888E-05	-0.000426	0.00041451	0.014074	0.99831894	1.027733239	0.000137452	0.000215
5	0	sample	4	TRUE	0.00035	0.0015	0.0005	backward	TRUE	8.1764E-05	-0.0007084	0.00086943	0.018016	0.997405337	0.814811232	0.000705521	0.000327
6	0	sample	5	TRUE	0.0001	0.0015	0.0005	backward	TRUE	0.00119814	0.00104519	0.00021999	0.062279	0.972082807	-4.751159409	1.2905E-05	0.000659
7	0	sample	6	FALSE	0.00025	0.0015	0.0005	backward	TRUE	1.6553E-05	-0.0012465	0.00106397	0.054271	0.981092276	1.171585964	0.000754686	0.000859

Figure 14. The OFET Summary sheet.

4. RESULTS AND CONCLUSION

The data from the anodization experiments was analyzed with the app. Each of the plots in Fig. 16 shows, for a particular anodization current, how the mobility estimates and threshold voltage estimates changed as the anodization time was varied. These plots were not made with the app, but were made with the estimates output

	A	B	C	D	E	F	G	H	I	J
1	Group	Grouped By	Number of Inliers	Number of Outliers	Threshold Voltage Estimate (V)	Threshold Voltage Error (V)	Mobility Estimate (m^2 / (V · s))	Mobility Error (m^2 / (V · s))	Hysteresis (1 / V)	Hysteresis Error (1 / V)
2	0	sample	4	8	1.081062128	0.32823981	0.000460877	0.000219082	0.00051001	0.000179794
3	1	sample	8	4	1.83402462	0.039468586	0.000869897	0.000213054	0.000851776	7.50713E-05
4	2	sample	11	1	1.83035767	0.034319223	0.000828032	0.000191069	0.00080407	5.99766E-05
5	3	sample	11	1	2.035581438	0.03613983	0.00070158	0.000166431	0.000624993	7.21408E-05

Figure 15. The Group Summary sheet.

by it. Each error bar represents the standard error of the corresponding estimate. The highest average mobility was observed in the devices processed with an anodization current of 0.4 mA and an anodization time of 400 sec.

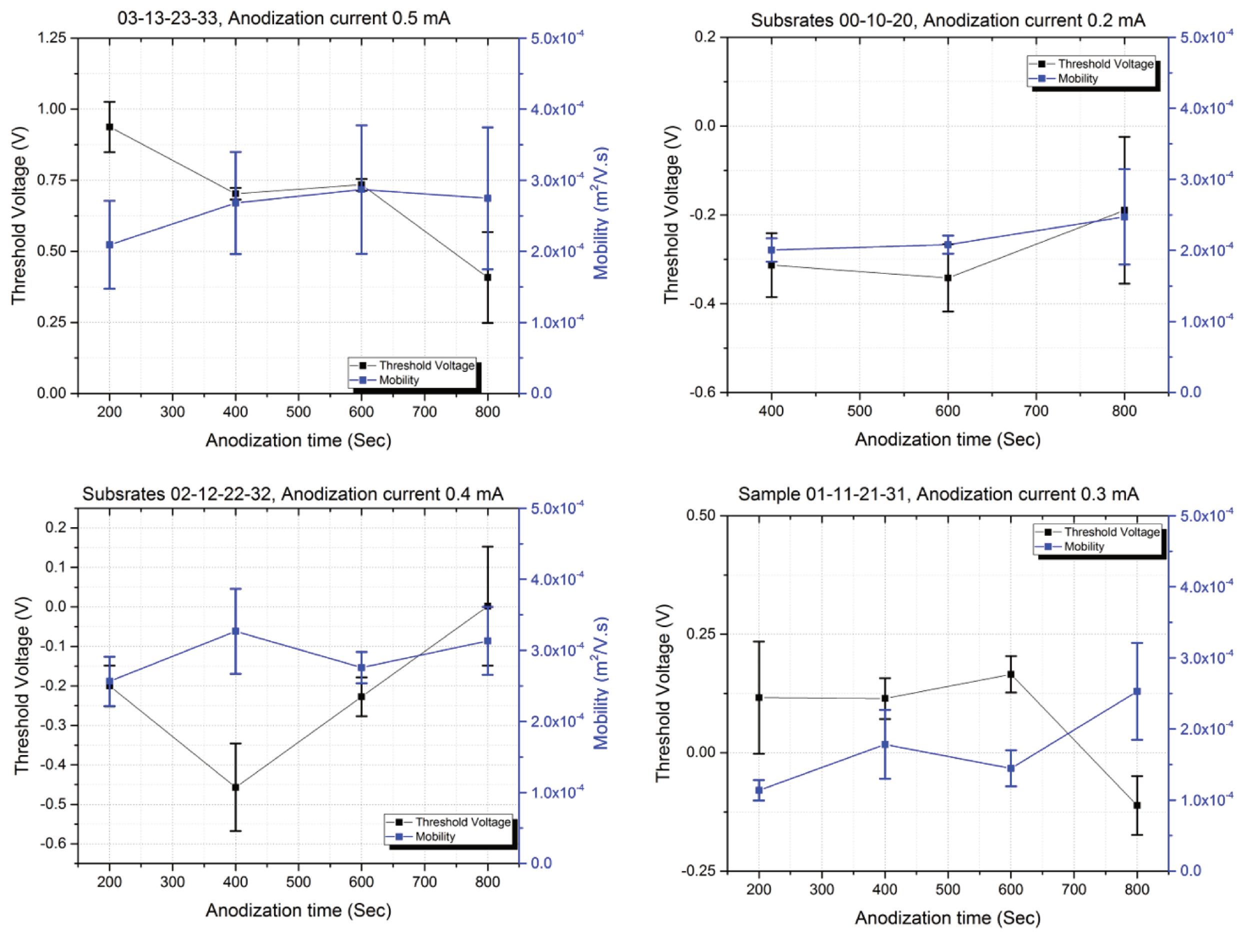

Figure 16. The variation in the mobility and threshold voltage of the devices with anodization time for the different anodization currents.

We have shown that our web application can be used to easily perform several of the steps in an analysis of OFET data. Once the user has uploaded a file with data from an experiment and entered information like the number of OFETs, many of the computations are carried out automatically. In particular, the estimation of the mobility and the threshold voltage are done automatically for each OFET and each group of OFETs. The estimation is done by fitting a nonlinear regression model to every sweep. This does not require the user to choose a gate voltage range over which to perform linear regression. The app does not fully automate the identification of outlier OFETs, but it does provide features that make identification simple and does automatically exclude outliers from calculations when necessary. Full automation of outlier identification would be unwise. No identification algorithm can be expected to perform with perfect accuracy on real-world datasets, so the user needs to have the ability to flag outliers themselves.

We are continuing to improve the app and add features to it. We have been investigating the possibility of using a cutoff for the normalized RSE or the pseudo-R^2 to aid in outlier identification. The outlier identification algorithm on the Outlier Flagging tab could be refined so that it performs better when the data is very messy, as it can be when the anodization conditions haven't been optimized. We have also been considering adding a feature that employs hypothesis testing to suggest which sweep type to use. The app was originally designed to process n-type OFET data and was extended so that it would also be able to process p-type OFET data. It could possibly be extended to have the ability to process data on other kinds of transistors, such as organic electrochemical transistors.

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