

# Generate Tafel Plots in AfterMath from CV or LSV Data

Illustrated Use of Basic Math Transformations

AfterMath can be used to convert cyclic voltammetry (CV) and linear sweep voltammetry (LSV) data from typical current vs. potential plots to Tafel Representations, such as potential vs. log current density. The steps to perform this transformation are documented here, but the process is still manual at the time this document was written.

## **1. Tafel Plot Formatting**

Tafel plots are a useful for evaluating kinetic parameters from electrochemical data. Tafel plots are only valid for electrochemically irreversible systems. In the field of electrochemical corrosion measurements, Tafel plots are used to extract anodic and cathodic slopes as well as corrosion potential and corrosion current.

AfterMath software includes data tools and transforms that convert current vs. potential data into Tafel form. AfterMath also provides tools to measure a linear baseline, such that  $\beta_a$  (anodic component slope) and  $\beta_c$  (cathodic component slope) can be obtained. These empirical values may be desired for subsequent calculations in Linear Polarization Resistance experiments, commonly used in the field of electrochemical corrosion.

At present, the process to produce a Tafel representation and subsequent data output is manual. AfterMath has been updated to include corrosion techniques, such as Linear Polarization Resistance (LPR), which uses Tafel slopes to calculate corrosion rates.



#### INFO:

Tafel Plot transformation requires taking the  $log_{10}$  of the absolute value of current (or current density) values. You must have AfterMath version 1.4.8863 or later installed for this transformation to operate properly. This version of AfterMath can be downloaded from <u>www.pineresearch.com</u>. Review the AfterMath Knowledgebase to find the download link.

# 2. Plot Transformation

## 2.1 Organize CV or LSV Data

Tafel plot representation of current vs. voltage data is easier to read for linear sweep (one segment) current vs. voltage data. If your data is already a single segment LSV, proceed to the Section 7.

If your data are a multiple segment CV (see: Figure 2-1), extract only the one segment of interest.

## 2.1.1 Removing a Segment from a CV

If required, remove a segment from the cyclic voltammogram, leaving only a linear sweep voltammogram. We recommend creating a new plot, such that the original data are preserved.

- 1. Right click the cyclic voltammogram trace in AfterMath.
- 2. Choose "Select points..."
- 3. Select the "Segments" radio button, then choose the segment you want to convert to a Tafel plot. Notice that doing so will highlight only the data for the chosen segment (see: Figure 2-1).

2741 Campus Walk Avenue | Building 100 | Durham, NC 27705 | USA Phone: +1 919.782.8320 | E-mail: pinewire@pineresearch.com | http://www.pineresearch.com



Figure 2-1. Selection of Only One CV Segment in AfterMath

- 4. Press OK.
- 5. Copy these data (Ctrl-C or right click  $\rightarrow$  copy).
- 6. Right click in the AfterMath archive and select New  $\rightarrow$  Plot.
- 7. Right click the blank plot that you just created and paste the data (Ctrl-V or right click  $\rightarrow$  paste).

Now you have extracted one segment of a CV to create a new one segment LSV plot (see: Figure 2-2).





## 2.2 Adjust Axes and Units as Desired

By default, AfterMath plots current (not current density) on the y - axis and potential on the x - axis. While this is fairly uniform across the electroanalytical community, the corrosion community typically reverses these axes. Prior to performing Tafel analysis, change any plotting orientations and units as desired.

## 2.2.1 Adjusting Plot Axes

The corrosion community typically plots potential on the x - axis and current (or current density) on the y - axis. This is a simple "Basic Math Operations" Transform in AfterMath.

- 1. Right click the LSV data on the plot and choose Apply Transform → Basic Math Operations... (see: Figure 2-3)
- 2. Select "Swap X/Y" Function. Ensure "Replace original trace" box is ticked under Options.
- 3. Press OK.

R

		Now	Diat			
	Basic Math Operations					
40.0	Function					
	O Addition (+)	O Inverse (1/x)	O Exponential (e*)	OL	ogarithm [Ln(x)]	
	O Subtraction (-)	O Square (x²)	O Exponential10 (10")	OL	ogarithm10 [Log(x)]	
-	O Multiplication (x)	◯ Square Root (√)	O Exponential (a*)	Ox	-Y Product	
	O Division (/)	O Absolute Value	O Negate	00	hange Unit	
	Swap X/Y	O Tafel log( x )				
0.0	Parameters					
0.0 -	Operand Value		Operand Unit Selection			
	Operand value.		Standard units		~	
	Operand Unit: Cu	Operand Unit: Current		0 🔹 /	1.0	
	Options	Options			1.5	
	Replace original to	Replace original trace     Omit out-of-bounds data points     Perform operation on Y-data only			1.5	
	Omit out-of-bou			0 +	1(4)	
	<ul> <li>Perform operation</li> </ul>			10 /	1.0	
	O Perform operation	n on X-data only	Temperature (K):	0 🔹	1.0	
			Molarity (mol):	0:	1 .	
			Luminosity (cd)	0 +	1 📮	
1			Angle (rad)	0 🔹	1.	
			Solid Angle (sr)	0 🔹	1.0	
0.0						
-750.0					OK Cancel	

Now potential will be on the x - axis and current will be on the y - axis.

Figure 2-3. Use of Basic Math Operations to Transform Axes

### 2.2.2 Plot x - axis as Current Density

Some scientists prefer to work in current density, which is simply the current divided by electrode area. By default, AfterMath does not perform this normalization and will always output current. With another simple "Basic Math Operations" Transform in AfterMath, current can be converted to current density.

- 1. Right click the LSV data on the plot and choose Apply Transform → Basic Math Operations... (see: Figure 2-4).
- 2. Select "Division (/)" Function.
- 3. Enter Operand Value (i.e. the electrode area, in  $m^2$ ).
- 4. Tick the "Replace original trace."
- 5. Choose the appropriate radio button to perform this operation on the x axis or y axis. Choose the axis displaying current.

- 6. Select "Area" from the Standard units dropdown in the Operand Unit Selection section.
- 7. Press OK.

R

			New	Plot					
250.0	E	Basic Math Operations							
0.0 -		Function Addition (+) Subtraction (-) Multiplication (x) Division (/) Swap X/Y	<ul> <li>○ Inverse (1/x)</li> <li>○ Square (x<sup>2</sup>)</li> <li>○ Square Root (√)</li> <li>○ Absolute Value</li> <li>○ Tafel log(x)</li> </ul>	<ul> <li>Exponential (e<sup>n</sup>)</li> <li>Exponential 10 (</li> <li>Exponential (a<sup>n</sup>)</li> <li>Negate</li> </ul>	) (10%) )	C Logar Logar X-Y Pi Chang	ithm [Ln(x)] ithm10 [Log(x)] roduct ge Unit		
Potential (mV)	æf	Parameters Operand Value: Operand Unit: Arr Options Replace original t Omit out-of-bou Perform operatio	2e-5 ea race nds data points n on Y-data only	Operand Unit Selec Standard units: Length (m): Mass (kg): Time (s): Current (A):	Area 2 0 0	• / _ • / _ • / _	× 1 + 1 + 1 + 1 + 1 + +	B	
-500.0 - - d <sup>2</sup>	<i>"</i>	Perform operation	n on X-data only	Temperature (K): Molarity (mol): Luminosity (cd): Angle (rad): Solid Angle (sr):	0		1 + 1 + 1 + 1 + * 1 + *		
-20.0						OF	Conset		40.0

Figure 2-4. Use of Basic Math Operations to Convert Current to Current Density

Change the units on the current axis by double-clicking the axis to open the Axis Properties window. Here, untick "Automatic unit selection" under the Units section and choose the desired units to display (see: Figure 2-5).

		New Plot	
250.0 ]			
	Axis Properties		
-	General	Units	
	Line color	Automatic unit selection	
0.0	Line width 1	• Units amp per square meter	~
0.0-	Position Bottom	V Metric prefix (None)	~
	Gridline Style	Automatic axis label with unit	
-	Color	- Cash	
	Width	Scale	
250.0	Tickmark Style	Auto 🖸	
230.0 7	Length 5		3
	Position - Outside		
-			
	Hidden	Label interval	1
500.0 -		Minor tickmarks	
/		Decimal places	*
1		OK Cancel App	ly .
750.0		· · · · · · · · · · · · · · · · · · ·	
-10	0	.0 1.0	3

Figure 2-5. Adjustment of Unit Display on a Plot in AfterMath

## 2.3 Convert to Tafel Plot (log current plot)

- 1. Right click the LSV data on the plot and choose Apply Transform → Basic Math Operations... (see: Figure 2-6).
- 2. Select "Tafel log (|x|)" Function.
- 3. Tick the "Replace original trace."
- 4. Choose the appropriate radio button to perform this operation on the x axis or y axis. Choose the axis displaying current.



#### INFO:

The current axis remains in scalar format. While the log of current has been taken, the axis will not be a logarithmic axis. You can manually edit the axis label to add "log" for clarity (see: Figure 3-1).



Figure 2-6. Use of Basic Math Operations to Transform Plot to Tafel Convention

The final result will be the correct form of a Tafel Plot (see: Figure 3-1). In real world systems, especially in the electrochemical corrosion field, the data may appear well-behaved, as shown in nearly all textbooks. Real-world systems may not always exhibit classic behavior. Realize the steps provided in this guide are simple arithmetic transformations and have not altered your data in any way. The transformations have only adjusted how the data are presented on a plot.

The next step is often to extract slope data for the anodic and cathodic components of the Tafel Plot, for use in corrosion rate calculations. Some users may simply use common estimates of these values, based on the corroding material. In other cases, researchers may wish to analytically determine the slope.

The next section will discuss how to extract the Tafel Slopes with simple tools.

## 3. Slope Determination

AfterMath includes a variety of tools for data analysis. The "Baseline" option is useful for finding the slope about a series of data points. The Baseline tool can be used to extract that  $\beta_a$  and  $\beta_c$  values from the transformed Tafel Plot from Section 1.



Figure 3-1. Tafel Plot Representation of Current vs. Voltage Data

## 3.1 Determine Tafel Slopes, $\beta_a$ and $\beta_c$

Once the Tafel plot has been created (from CV or LSV data, as above), use the Baseline tool to find the slope about a section of data, selected by the user.

	INFO:
i	AfterMath will place colored dots and a dashed baseline onto the data. By default, AfterMath performs a regression fit about the data between the two pink dots. Double click the pink dots to open the tool properties window, where the Baseline Mode can be changes to suit (Regression recommended).
	The dashed black line and black dots are simply a straight baseline drawn for visualizing the line from which the slope and intercept are calculated.

- 1. Right click the LSV data on the plot and choose Add Tool → Baseline(see: Figure 3-2).
- 2. Adjust the two pink dots to the desired region of the curve where the slope should be calculated. The slope and intercept are calculated with each movement of the pink dots. Double click the label for additional (but not required) options for formatting and display options of the tool results.
- 3. Repeat Steps 1 2 for the other slope on the Tafel Plot.

The Tafel Plot with slope determination is now complete (see: Figure 3-3). Adjust the view of the plot by doubleclicking axes and manually setting the maximum, minimum, and label interval for optimal viewing.

Record the slope values for further use and calculations as needed. Saving the archive preserves all of the transformations and analyses performed and can be referenced at a later point.



Figure 3-2. Addition of Baseline Tool to Tafel Plot for Slope Determination



Figure 3-3. Tafel Plot with Slope Measurements (axes optimized for best data view)

## 4. Contact Us/Support

Our offices are located in Durham, NC in the eastern US time zone. We are available by phone Monday through Friday from 9 AM EST to 5 PM EST. You can reach a live person by calling +1 (919) 782-8320. Alternatively, you may send an email to <u>pinewire@pineresearch.com</u> for technical and sales support. Our goal is to respond to emails within 24 hours of receipt.