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# Practical Guides to Foot-of-the-Wave Analysis (FOWA) and Catalytic Tafel Plots Through Interactive Web Interface

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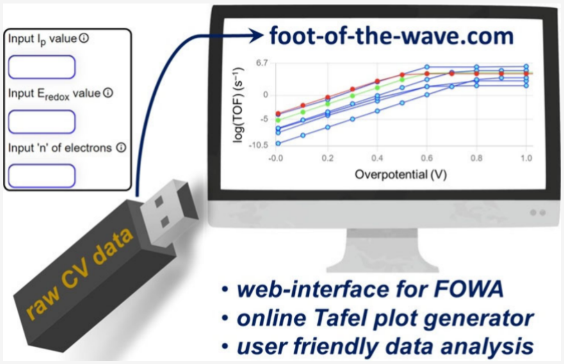
**ABSTRACT:** Analysis of cyclic voltammetry data has become essential to gain kinetic insights into electrocatalytic reactions, particularly in the field of small molecule activation. In such studies, the shapes of redox waves of the cyclic voltammograms are informative to distinguish between the catalytic and noncatalytic reactions. Kinetic parameters such as turnover frequencies (TOFs), rate constants, etc. can be extracted from the catalytic current−potential profiles. "Foot-of-the-wave" analysis (FOWA) is one such analysis, proposed by Savéant and Costentin, that provides kinetic information on electrocatalytic reactions. Although FOWA has been explained by many others, performing such analysis in practice, especially for new learners, is often intimidating. We present our recently developed web interface that provides a more flexible, reliable, and user-friendly platform for performing FOWA. We also provide step-by-step guidelines and training modules for studying FOWA that could help learners find the rate constant of the electrocatalytic reaction. Furthermore, our web design also provides opportunities to construct comparative catalytic Tafel plots, which are typically used to compare the *TOF*-overpotential relationship among the catalysts. We have also put efforts into building a database of the kinetic information for reported molecular electrocatalysts; primarily for the electrochemical carbon dioxide reduction reaction and hydrogen evolution reaction. The database can be further extended to other disciplines in electrocatalysis in the future. Overall, we believe that this web platform would benefit the global electrochemistry community, especially aspiring FOWA learners.



**KEYWORDS:** *Upper-Division Undergraduate, Graduate Education/Research, Analytical Chemistry, Inorganic Chemistry, Computer-Based Learning, Distance Learning/Self Instruction, Internet/Web-Based Learning, Electrochemistry, and Foot-of-the-wave analysis*

## 1. INTRODUCTION

Benchmarking molecular electrocatalysts for fuel-forming reactions such as hydrogen ($H_2$) evolution reaction, the production of hydrocarbons ($C_nH_{2n+2}$) by reducing $CO_2$, or the reduction of $O_2$/oxidation of $H_2O$ in the fuel cells (Box 1) has been an overwhelming research topic over the past decade.[1−8] These fuel-forming reactions require the control supply of multiproton and multielectron. The performance of those electrocatalysts is commonly assessed by comparing the catalytic plateau currents observed in the cyclic voltammogram.[3] However, side phenomena such as substrate depletion, deactivation of the catalyst, or product inhibition during the electrocatalytic reactions often impede the catalytic currents from reaching the ideal plateau;[9] therefore, obtaining accurate turnover frequency for an electrocatalytic reaction is sometimes not reliable based on the catalytic peak currents using the Randles-Sevcik equation.[10] Such challenges can be overcome using "foot-of-the-wave analysis" (FOWA) applied to cyclic voltammetry (CV) data.[9]

Many good explanations and concise summaries of FOWA are available in the literature,[3,11] however, we believe that web-based tools with systematic directions could benefit the researchers or learners of the electrochemistry community to perform FOWA hassle-free. Being motivated by the applications of FOWA in electrocatalysis and the need for such web platforms, we designed and developed a web interface, https://foot-of-the-wave.com/, that can perform FOWA using CV data. Our developed web interface can guide users to perform kinetic analysis for homogeneous electrocatalysis that are involved with multielectron and multiproton transfer reactions. The users are not required to have any programming skills to use the web tools. Rather we provide a Javascript-powered system that allows users to input their experimental parameters: peak currents, redox potential where the catalysis occurs, and the number of electrons

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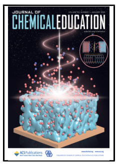

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**Box 1. Examples of fuel-forming reactions**

- $H_2$ evolution reaction
  - $H_2$ could be the “fuel for the future”

$$2H^+ + 2e^- \rightleftharpoons H_2$$

- $CO_2$ reduction reaction
  - formation of hydrocarbons (liquid fuels)

$$CO_2 + 2H^+ + 2e^- \rightleftharpoons CO + H_2O$$

$$nCO + (2n+1)H_2 \rightleftharpoons C_nH_{2n+2} + nH_2O$$

- $O_2$ reduction/$H_2O$ oxidation reaction
  - takes place in fuel cells

$$O_2 + 4H^+ + 4e^- \underset{\text{oxidation}}{\overset{\text{reduction}}{\rightleftharpoons}} 2H_2O$$

involved in the catalysis. The programming code will use those inputs and process the users’ uploaded CV data to provide the reaction rate constant ($k_{FOWA}$). It is worth noting that such $k_{FOWA}$ could be the rate constant for the first chemical step in a multistep catalytic cycle or equal to a rate constant ($k_{cat}$) for the overall electrocatalytic reaction if the first chemical step is the rate-determining step.[12] However, appropriate regions associated with the “foot” of the current−potential curve need to be chosen to estimate the $k_{FOWA}$ value, and our web-based tools allow users to make multiple attempts to find the best “foot” according to their preferences. To guide the users in finding the appropriate “foot” and the significance of the FOWA, we provide a short tutorial herein.

Furthermore, it is common practice to compare the rate of the electrocatalytic reaction with its reported counterparts by constructing catalytic Tafel plots.[1,13] In our designed web interface, users can construct Tafel plots by selecting the reported catalysts of interest from our database, which contains a library of references for the reported molecular electrocatalysts for multiproton and multielectron molecular electrocatalysis, particularly for the $CO_2$ reduction reaction ($CO_2RR$) and $H_2$ evolution reaction (HER), by gathering their reported $k_{cat}$ values and operating conditions. The objective of the website and this article is to provide a platform whereby users can find the catalysts of their interest from the literature to generate a comparative Tafel plot for benchmarking their catalysts online in a faster, more reliable, and more flexible way.

## 2. REQUIRED CONCEPTS TO PERFORM FOWA

### Understanding Voltammetric Responses for Kinetic Analysis

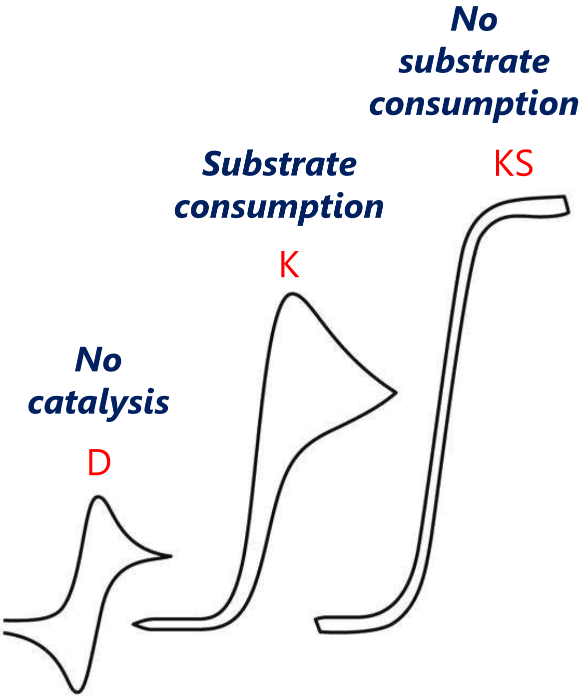
The fundamentals of the CV technique, including the practical guides and CV data interpretation, have been well demonstrated to train students interested in electrochemistry.[10,14−16] However, the CV responses for molecular electrocatalysts should be well-diagnosed prior to kinetic analysis. Savéant and co-workers have explicitly mapped out the different CV responses in a kinetic zone diagram with a model example of one-electron redox catalysis.[17] Their model examples consider that a molecular catalyst P can be reversibly reduced to Q, and Q then reduces substrate *A* with one electron to product *B* and regenerates catalyst *P* (Box 2). Thus, the overall electrochemical mechanism becomes $E_rC_i$, where $E_r$ is the step for the reversible redox couple of *P*/*Q* (the electrode supplies the $e^-$), and $C_i$ is the rate-limiting step which is the homogeneous $e^-$ transfer from *Q* to *A*. Therefore, the CV response for the first $E_r$ step is reversible (Box 2, *no catalysis*, *D* zone).[17] Next,

**Box 2. Model 1e⁻ Redox Catalysis**

$$P + e^- \overset{E_r}{\rightleftharpoons} Q$$

$$Q + A \xrightarrow{C_i} P + B$$

**CV responses:**



D: Reversible redox couple for P/Q

K: Q reduces A, but the concentration of A at the electrode is less than that in the bulk during reverse scan, indicating *substrate consumption.*

KS: Q reduces A, but the concentration of A is the same at the electrode and in the bulk – *no substrate consumption.*

CV traces are adapted from ref 2 and modified. Copyright 2017 Springer Nature.

suppose the reduction of substrate $A$ is possible at the potential where the $P/Q$ couples; an irreversible CV with the increase in reductive peak current will show up upon the addition of $A$. The shape of the catalytic CV trace depends on the concentration of substrate $A$ at the reaction-diffusion layer (RDL) − the interface between the electrode surface and the bulk solution. If the concentration of $A$ at the electrode is equal to that in the bulk solution, indicating no substrate consumption in the RDL during the electrocatalysis, the CV should ideally be "S-shaped" (Box 2, KS zone). This catalytic phenomenon is classified as the pure kinetic condition for redox catalysis, and the plateau current ($i_{\text{pl}}$) can be used to obtain $k_{\text{cat}}$ (Box 3).

**Box 3. Equations Used for the Rate Constants if Plateau Currents Observed**

$$i_{pl} = nFA[cat]\sqrt{Dk_{cat}},\ \text{Eq. (1)}$$

$$\frac{i_{pl}}{i_p} = \frac{n}{0.4463n'}\sqrt{\frac{RTk_{cat}}{n'Fv}},\quad \text{Eq. (2)}$$

| | |
|---|---|
| $i_{pl}$: | Plateau current in catalytic CV |
| $i_p$: | Peak current observed in the absence of substrate |
| $n$: | Number of electrons participated in the electrocatalysis |
| $n'$: | Number of electrons transferred from the electrode to the catalyst in the absence of substrate |
| F: | Faraday constant (96,485 C/mole) |
| A: | Geometric surface area of the electrode ($cm^2$) |
| $[cat]$: | Concentration of the catalyst in the bulk solution ($mol/cm^3$) |
| D: | Diffusion co-efficient measured for the catalyst ($cm^2/s$) |
| R: | Gas constant (8.3145 J $mol^{-1}$ $K^{-1}$) |
| T: | Temperature (K) |
| $v$: | Scan rate (V/s) |
| $k_{cat}$: | Rate constant ($s^{-1}$) |

However, if A is consumed in the RDL during the catalysis, then the reverse CV scan does not overlay with the forward scan, and a peak-shaped CV is observed (Box 2, substrate consumption, $K$ zone). Accounting for the peak currents in the forward scan to obtain the kinetic information is not trustworthy for these peak-shaped CVs. For these cases, FOWA is useful to estimate the reaction rate constants. The basic assumption for the FOWA is that the current response at the "foot" of the catalytic CV experiences negligible perturbation by side phenomena such as substrate consumption or catalyst deactivation. Ideally, the initial segment of the catalytic CV wave (the "foot") that is between the onset potential ($E_{\text{onset}}$) and the half-wave potential ($E_{\text{cat/2}}$) is used for the FOWA; therefore, it is important that no additional redox events are present at the foot of the catalytic CV to extract accurate reaction rate constants.

## Finding the Appropriate Kinetic Analysis for Ideal and Nonideal CVs

We herein focus our discussion on the kinetic analysis for two typical catalytic CV waveforms − (1) S-shaped (ideal, KS zone, Box 2) and (2) peak-shaped (nonideal, K zone, Box 2) that have been well-investigated theoretically for the FOWA.[11,18,19] For the S-shaped CV, the plateau current can be directly used in eq 1 or eq 2 (Box 3), and the overall rate constant ($k_{\text{cat}}$) for electrocatalysis can be extracted (Box 3). Noteworthy, eq 2 is comparatively accessible to use, as it is independent of the catalyst concentration and diffusion coefficient of the catalyst.

## Foot-of-the-Wave Analysis for Nonideal CVs

The peak-shaped CVs should be treated differently for kinetic analysis. As the side electrochemical phenomena such as substrate depletion impede the formation of the plateau shape in the catalytic CVs, the foot of such CVs is considered for the analysis. The assumption behind such a consideration is that the current response should be identical at the foot of the peak-shaped CV and S-shaped CV as the effects of those side phenomena are less influential in that early segment of the CV trace. As the analysis at the foot of the catalytic CV wave is limited at the initial part of the CV, the reaction rate constant ($k_{\text{FOWA}}$) obtained for the nonideal peak-shaped CV only can be associated with the first chemical step. If the first chemical step is the rate-limiting step for overall redox catalysis that determines the rate of the product formation, $k_{\text{FOWA}}$ can be considered $k_{\text{cat}}$ for a multielectron, multiproton reaction. Noteworthy, the $k_{\text{cat}}$ values obtained from the FOWA are typically larger than the rate constant measured upon performing the bulk electrolysis, as FOWA assumes that no side phenomena occur during the catalysis.[3]

## Procedure for FOWA and Calculation for the Rate Constant

The applied potential window used in the CV studies is transformed into another function of potential, $[1+e^{\{F(E-E_{cat/2})/RT\}}]^{-1}$, where $E_{\text{cat/2}}$ is the potential at which half of $i_{\text{pl}}$ is reached (Figure 1). The window of $[1+e^{\{F(E-E_{cat/2})/RT\}}]^{-1}$ is then plotted versus the ratio of the catalytic peak currents ($i_{\text{cat}}$) observed in the peak-shaped CVs to the peak currents ($i_{\text{p}}$) in the absence of a substrate (Box 4). The catalytic current ($i_{\text{cat}}$) used for the FOWA should be considered after subtracting the background currents, typically obtained by running the CV in the absence of the catalyst under the catalysis conditions. Such background current corrections are necessary to gain more accurate kinetic information based on the actual catalytic current near onset potentials by neglecting the amount of current due to the bare electrode contribution. However, upon fitting using the FOWA eq (eq 4, Box 4), a sigmoidal graph should be obtained, and as mentioned earlier, the portion of the sigmoidal graph that corresponds to the range of the potentials between onset and $E_{\text{cat/2}}$ should be fitted linearly to obtain the slope value. This slope value will provide the reaction rate constant $k_{\text{FOWA},}$ according to eq 4, shown in Box 4.

## Interpretation of Rate Constant Obtained from FOWA

Supposing the entire potential window between the onset and $E_{\text{cat/2}}$ in the voltammogram becomes linear upon fitting the

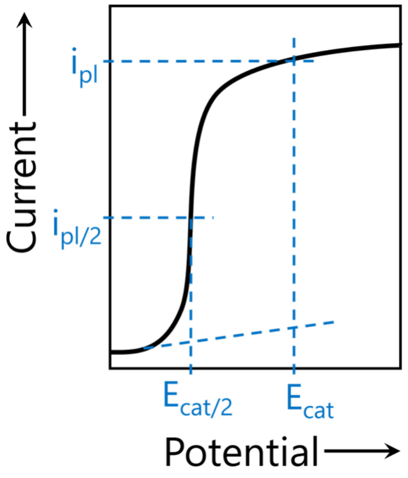


**Figure 1.** A model "S-shape" catalytic CV with the typical notations used to define the plateau current ($i_{pl}$) and catalytic potential ($E_{cat}$), and their measure at the half-wave as $i_{pl/2}$ and $E_{cat/2}$.

**Box 4. Equations Related to FOWA**

$$\frac{i_{cat}}{i_p} = \frac{i_{pl}/i_p}{1+e^{[f(E-E_{cat/2})]}} \qquad \text{Eq. (3)}$$

$$\frac{i_{cat}}{i_p} = \frac{2.24\frac{\sqrt{k_{FOWA}}}{\sqrt{fv}}}{1+e^{[f(E-E_{cat/2})]}} \qquad \text{Eq. (4)}$$

$i_{cat}$: Catalytic peak current

$f$: F/RT ($V^{-1}$)

$k_{FOWA}$: Rate constant ($s^{-1}$) obtained from FOWA

$E$: Applied potentials (V)

$E_{cat/2}$: Potential (V) at half-wave

Note: $i_{pl}$, $i_p$, F, R, T, and $v$ are the same as defined in **Box 3**.

FOWA eq 4 in Box 4 (Figure 2, KS zone), such linearity indicates that the first chemical step is the rate-limiting step and therefore, $k_{FOWA}$ obtained from the FOWA slope, as discussed in the previous paragraph, suggests the overall catalytic reaction $k_{cat}$ or the maximum turnover frequency ($TOF_{max}$) of the catalysis of interest.[20] Ideally, such estimated $k_{cat}$ or $TOF_{max}$ should be close to the value of $k_{cat}$ obtained using eq 1 (Box 3) if the plateau current, $i_{pl}$ is observed in CV. On the contrary, if the potential window between the onset and $E_{cat/2}$ deviates from the linearity (Figure 2, K zone), the best linear fit will provide the reaction rate constant of the first chemical step of a multistep redox catalytic reaction.

## 3. WEB INTERFACE DESIGN FOR FOWA

Our web design comprises four navigation tabs, "Introduction," "Manual," "FOWA," and "Tafel." The tab "Introduction" briefly describes the FOWA and Tafel equations and also guides users on how to determine the parameters, such as catalytic current, catalytic potential, overpotential, etc., from cyclic voltammograms. The second tab "Manual" guides the users about the requirements of the inputs and how to prepare the files before uploading them to the website and provides the step-by-step procedures for the use of our website with snapshots of some of the model results. The next navigation window "FOWA" processes the uploaded file containing the CV data and such a tab is sketched by following the steps, as described in Figure 3. In the "FOWA" tab, the required inputs are $i_p$, catalysis potential ($E_{redox}$), and number of electrons (n) involved in catalysis (Figure 3A). The CV data then need to be uploaded with the required extension, as described in the "Manual" window (Figure 3B). Using those inputs, JavaScript will process the uploaded file and display a sigmoidal trace output on the screen (an example trace is shown in Figure 3C). The user can then select any two points in that sigmoidal trace,

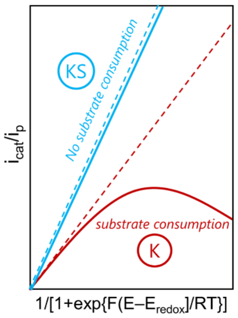


**Figure 2.** A model example of FOWA performed for an S-shaped CV (blue) and a peak-shaped CV (red). The dotted lines indicate the linear fitting of the model FOWA traces. The fitted line matches with the FOWA trace when there is no substrate consumption (KS zone, corresponding to the S-shaped CV), but deviates from the FOWA trace if there is substrate consumption (K zone, corresponding to the peak-shaped CV).

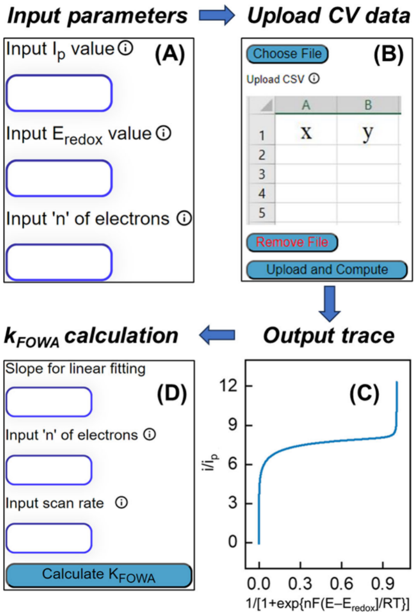
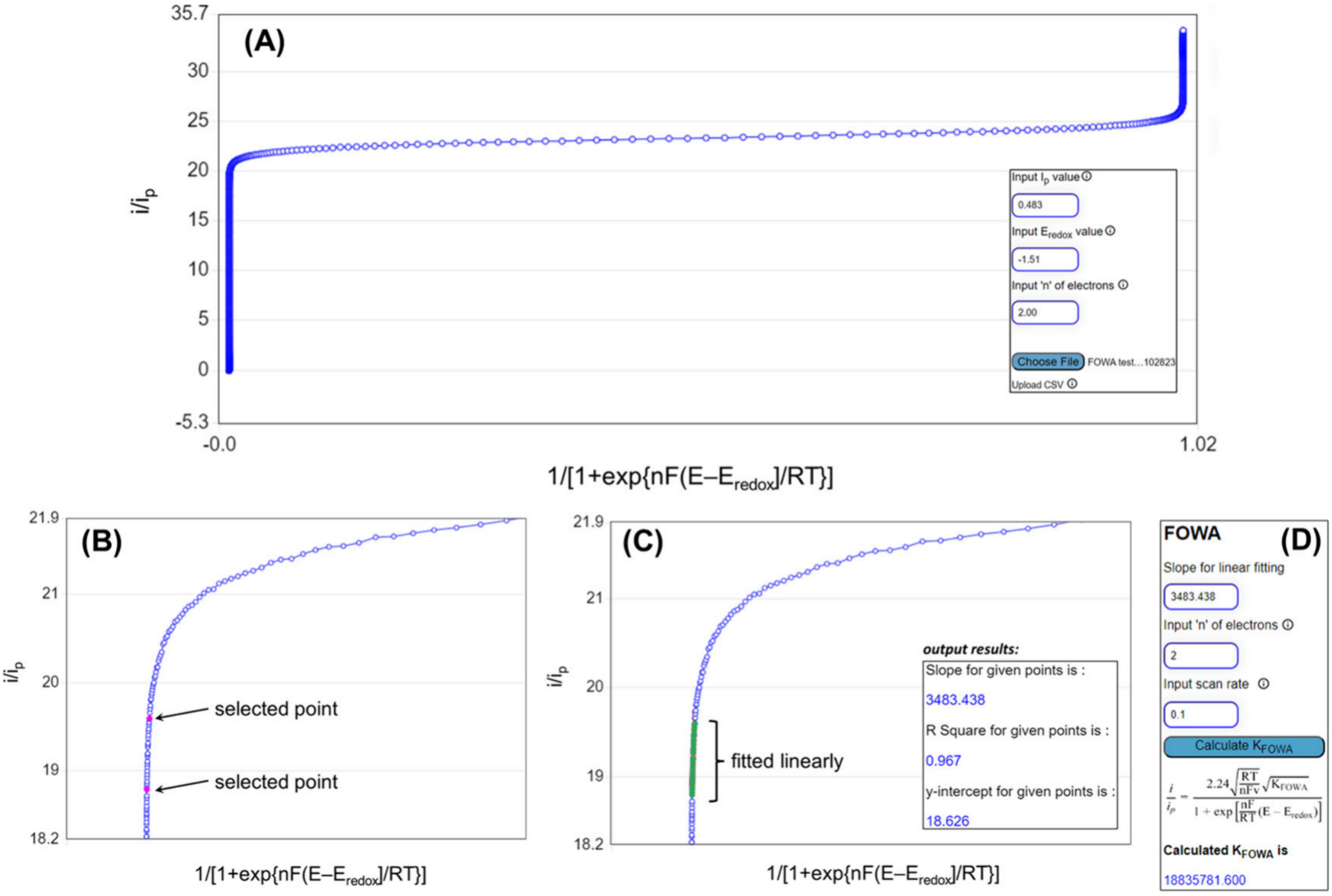


**Figure 3.** A step-by-step guide to operating the web tools and the expected output trace for FOWA.



Input $I_p$ value
0.483

Input $E_{redox}$ value
-1.51

Input 'n' of electrons
2.00

FOWA test…102823

Slope for given points is : 3483.438

R Square for given points is : 0.967

y-intercept for given points is : 18.626

Slope for linear fitting
3483.438

Input 'n' of electrons
2

Input scan rate
0.1

Calculated $K_{FOWA}$ is 18835781.600

**Figure 4.** (A) A sample FOWA trace generated by our designed web interface using $i_p = 0.483$, $E_{redox} = -1.51$, and $n = 2.00$ (inset). (B) Selected points between $E_{onset}$ and $E_{cat/2}$ corresponding to the "foot" of the CV are shown with pink dots. (C) The green region indicates the portion of the FOWA trace selected for the linear fitting and the fitting parameters (inset). (D) A screenshot from the FOWA tab of our developed web interface where the slope value obtained from the FOWA fitting can be used to calculate the rate constant ($k_{cat}$). The supporting raw CV data file tested to generate these FOWA traces is provided as a separate document file.

preferably near the origin of the coordinates, to ensure that the selected data points lie between the respective $E_{onset}$ and $E_{cat/2}$ of the CV "foot". The web tools then perform the linear fit using that selected window and yield the slope of the linearity with the $R^2$ value (the coefficient of determination in a regression model). For an acceptable slope value to estimate the $k_{FOWA}$, the $R^2$ value should be >0.95. If users are satisfied with the linearity of the fitted curve, they can proceed to the next step to compute the $k_{FOWA}$. Under the same navigation window, "FOWA," the users need to fill out the obtained slope, the number of electrons in catalysis, and the scan rate at which the CV trace was obtained (Figure 3D). Finally, clicking on the "Calculate $K_{FOWA}$" button (Figure 3D) will show the rate constant, $k_{FOWA}$, of the electrochemical reaction.

## 4. OPERATION AND VALIDATION OF FOWA USING WEB TOOLS

Our programming code will execute eq 4 (Box 4) to generate the FOWA traces from the users' uploaded files and given parameter inputs. We have performed a few test runs using our designed web interface, and the obtained FOWA traces are shown in Figure 4 (see supporting file for the raw CV data used to generate this trace). Figure 4A shows a typical FOWA trace that can be obtained from our developed web interface. For the purpose of the demonstration, two random points that lie at the "foot" of the catalytic CV diagram have been chosen (Figure 4B) and fitted linearly to get the slope value (Figure 4C). To obtain the rate constant, the user needs to copy and paste these slope values into the designated box (a screenshot is provided in Figure 4D) on the same tab of the web page that displays the rate constant. To test the accuracy of our web tools, we performed FOWA for our previously reported electrochemical $CO_2$ reduction reaction[21] using our designed website and obtained the rate constant of the overall catalysis as $1.49 \times 10^5$ $s^{-1}$, which is close to our previously reported value, $1.41 \times 10^5$ $s^{-1}$, estimated by performing FOWA with the traditional manual data analysis strategies.

## 5. LIMITATIONS IN OUR DESIGNED WEB INTERFACE

The electrochemical mechanism for the catalysis of interest should be understood before performing FOWA as the equations of the $i_{pl}$ and $E_{cat/2}$ are mechanism-dependent.[22] Typically, for multielectron and multiproton reactions (as shown in Box 1), the electron transfer (E) and proton transfer (C) events occur in a particular sequence. For example, the transfer of 2 protons and 2 electrons during the electrochemical reduction of a substrate can occur in the following fashions, EECC, ECEC, or ECCE. If these E steps occur at the electrode surface, the processes are called heterolytic.[12] On the contrary, if the E steps are involved in the dimerization of the redox species in the solution, they are called homolytic reaction processes.[12] Noteworthy, eq 4 (Box 4) is only applicable for the EECC, ECEC, or ECCE mechanisms, and our developed web tool for performing FOWA does not work for other electrochemical mechanisms that are involved with disproportionation steps, homolytic processes, or catalytic reactions that are second (or higher)-order in catalyst concentration. Additionally, we have included the ECCE mechanism only for those cases where the second electron transfer is more thermodynamically favorable than the first electron transfer.

## 6. TAFEL PLOTS

The construction of catalytic Tafel plots is typically used to benchmark redox catalysts according to their intrinsic properties, regardless of experimental conditions.[1] TOF, theoretically defined as the moles of product produced per moles of the catalyst per unit time, is usually used to benchmark the kinetic behavior of catalysts.[9] However, for electrocatalysis, obtaining TOF within a certain potential window is comparatively more challenging but can be estimated by using eq 5 if the rate constant of the rate-limiting step (described as $k_{cat}$ or $TOF_{max}$ herein) is known from the FOWA. In catalytic Tafel plots, the plateau portion of the Tafel plots indicates the rate constant of the rate-limiting step that also could be the $TOF_{max}$. Furthermore, the TOF values within a potential (or overpotential) window can be estimated from the Tafel plot by using eq 5. The relation between the $TOF$ and the overpotential ($\eta$) for each catalyst of interest is plotted in a single Tafel diagram. The theoretical $TOF$ at different applied potentials also can be calculated by using eq 5, where the variables are the same as mentioned for the FOWA.[9] If the plateau current, $i_{pl}$ is observed in CV, the estimated $k_{cat}$ or $TOF_{max}$ obtained from the FOWA should match with the theoretical $k_{cat}$ value obtained by using eq 1 (Box 3), as the appearance of the plateau current suggests pure kinetic conditions without any side reactions, e.g., catalyst deactivation, cosubstrate inhibition, etc., that could limit the reaction rate.[11] Ideally, the theoretical and experimental TOF should match if 100% of the electroactive species on the electrode surface are active for the catalysis.

$$TOF = \frac{TOF_{max}}{1 + \exp\left(\frac{F}{RT}(E - E_{cat/2})\right)\exp\left(-\frac{F}{RT}\eta\right)} \qquad (5)$$

A comparative model catalytic Tafel is shown in Figure 5 for two different catalysts, $A$ and $B$, where catalyst $A$ is the better catalyst since it shows higher $TOF_{max}$ at a lower overpotential than that of catalyst $B$. The Marcus theory explains that the thermodynamic factors could influence the kinetics of the electron transfer processes.[23] In practice, higher $TOF$ comes at the cost of higher overpotential or vice versa.[1]

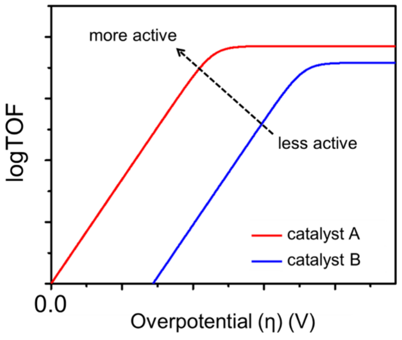


**Figure 5.** A model catalytic Tafel plots for benchmarking different catalysts for their catalytic activities for redox catalysis.

### Construction of Tafel Plots Using Our Web Tools

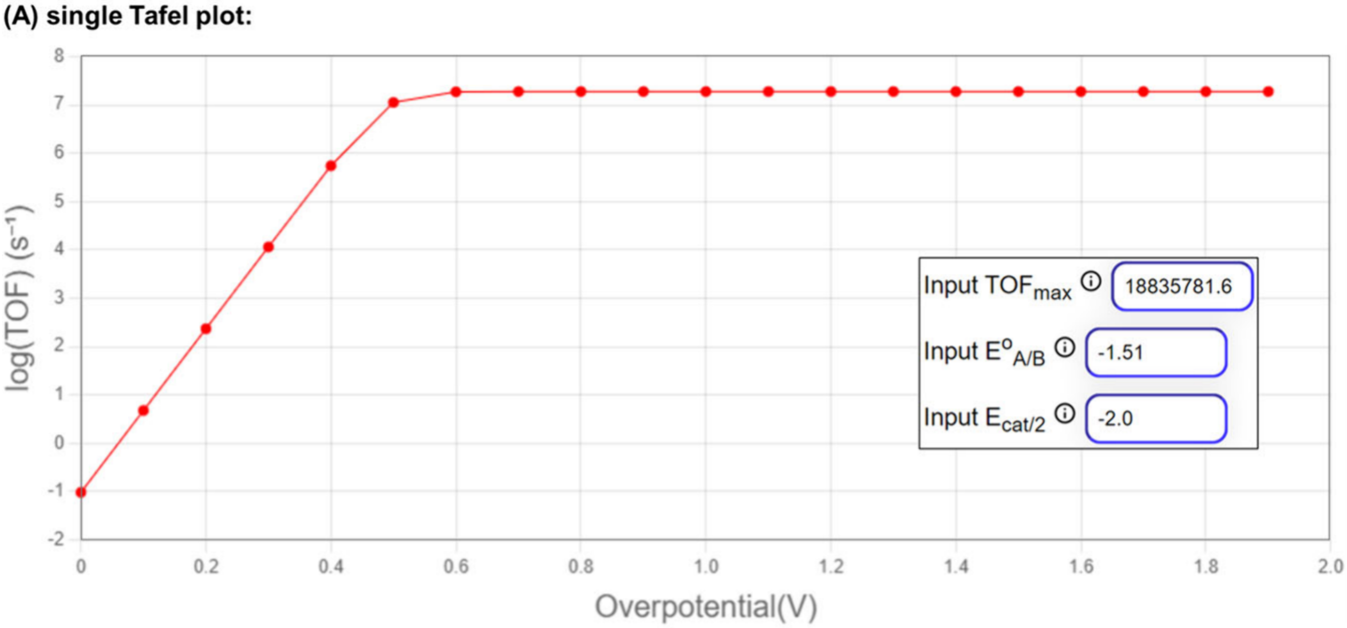
Accounting for the concept of catalytic Tafel plots, we provide an online function in our designed web interface to construct Tafel plots. In order to construct the Tafel plots, users need to provide only three inputs, the maximum $TOF$ ($TOF_{max}$) obtained for a catalytic reaction, $E_{redox}$, and $E_{cat/2}$ (Figure 6A inset). Clicking the option on the screen, "Generate Tafel Graph", after fulfilling these input requirements will show a single Tafel plot (an example is shown in Figure 6A). Herein, we have constructed a model Tafel plot (Figure 6A) by considering the $TOF_{max}$ (Figure 6A inset) which was obtained after analyzing the model FOWA, as shown in Figure 4D. The construction of catalytic Tafel plots is typically used to benchmark redox catalysts according to their intrinsic properties, regardless of the experimental conditions. Our web design provides the scopes to compare a single Tafel plot obtained for a catalyst of interest with the reported catalysts. To do so, the task is to select the choice of metal center, solvent, ligand, and proton source (Figure 6B inset). We have built up a library of references by noting the catalyst structures, operating conditions, TOF, and $\eta$. The web-based tool will extract the traces with matching parameters from the database to construct the Tafel plots and display them in the same graph so that their TOF-$\eta$ relationship can be well compared. An example of comparative Tafel plots is shown in Figure 6B.

### Building Database for Tafel Plots

We have gathered $TOF_{max}$ and $\eta$ values for the reported molecular electrocatalysts which are known for homogeneous $CO_2$RR and HER. On-screen, the users could navigate our database by selecting the metal center at the catalyst's active site, the solvent system in which the catalysis has been performed, coordinating ligand with the metal center, and the additional proton sources, which are typically added to the bulk solution to enhance the kinetics (Figure 6B inset). Although our recent database is limited to a few options under such categories, it will be updated regularly and maintained as new reports are available. We believe that such a library of literature will provide easy access to users to find the catalysts related to their research of interest and compare the $TOF$-$\eta$ activities, regardless of the reaction conditions. Furthermore, we also integrate the function of taking a "Graph Snapshot" of the Tafel plots that users can save on their systems.

## 7. INCLUSION IN UNDERGRADUATE AND GRADUATE COURSE CURRICULUM

We believe that the concept of FOWA can be included in upper-division undergraduate- and graduate-level courses. In such advanced-level courses, the electrochemistry syllabus is typically limited to finding half-cell reactions, balanced net redox reactions, interpretation of the voltammograms, and derivation of the equations. As the applications of electrochemical concepts are becoming wider in the current research trend, especially in the field of electrocatalysis related to energy, the environment, and sustainable chemistry, benchmarking the catalytic activities based on the reaction rates or turnover frequencies is very important. We believe the inclusion of newly developed concepts such as FOWA in the advanced level course curriculum and providing proper



Input $TOF_{max}$ ⓘ 18835781.6

Input $E^{o}_{A/B}$ ⓘ -1.51

Input $E_{cat/2}$ ⓘ -2.0

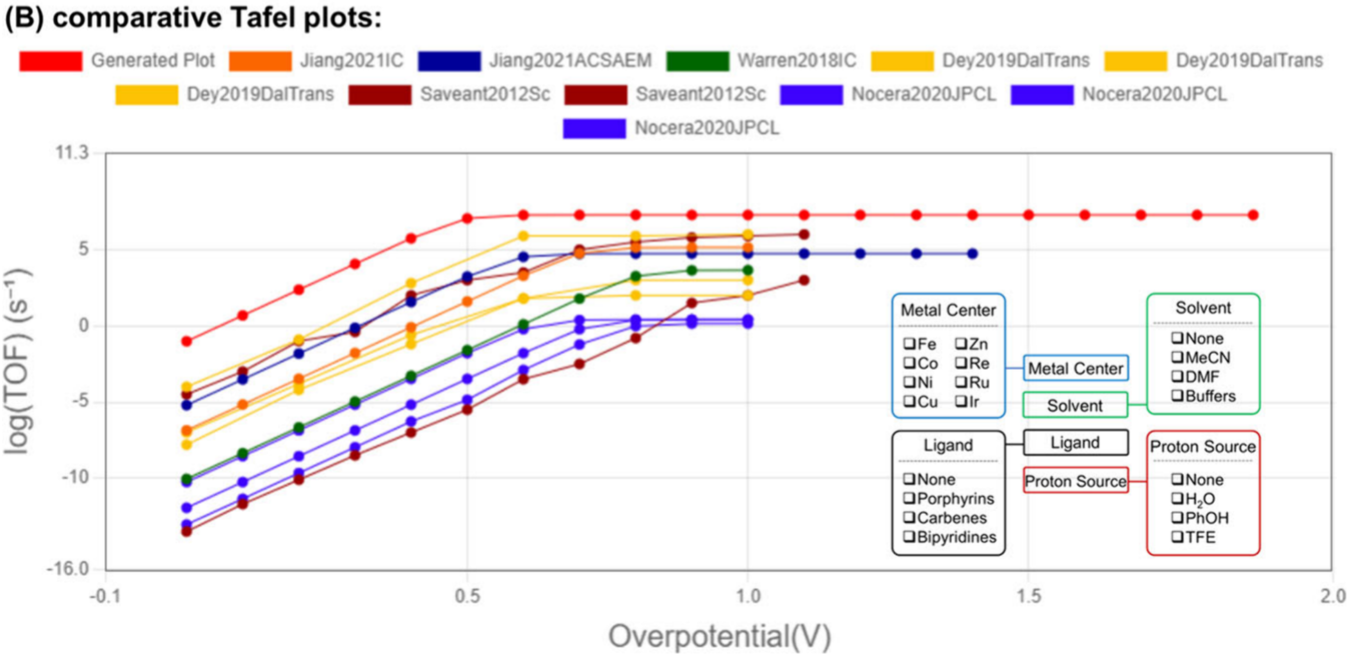


**Figure 6.** (A) A model catalytic Tafel plot (red) generated using our designed website and the required parameters (inset). (B) Comparative catalytic Tafel plots were also plotted by extracting the kinetic parameters from the database of our designed web interface.[21,24−29] The inputs given to our website were Metal center: Fe, Solvent: MeCN and DMF, Ligand: Porphyrins and Bipyridines Proton Source: $H_2O$, PhOH, and TFE (inset).

training will make students' backgrounds more competitive and also keep them more updated with the current research trend. To test the opportunities that our developed FOWA website could provide to the students learning of reaction kinetics of electrocatalytic reactions, we recently taught the FOWA in the advanced-level Analytic Chemistry II course. Students were given raw CV data for a catalytic $2H^+/2e^-$ reduction of $CO_2$ using a Fe-porphyrin catalyst and the required experimental parameters (such as $E_{redox}$, $E_{cat/2}$, $i_p$, scan rate, etc.) for performing FOWA, and asked to estimate the $k_{FOWA}$ from the FOWA trace by using our web design (see Supporting Information for the teaching modules used in the class). Students successfully executed the FOWA and reported their results by taking a screenshot of the web page. Some of the examples of the students' reports are shown in the Supporting Information. Furthermore, students also had the opportunity to construct a Tafel plot using our web interface to compare their estimated reaction rate constant with the reported catalysts for $CO_2$-to-CO conversion reactions. For such practices, students freely selected the solvent systems, metal center, ligand system, and proton source according to their choices and reported the comparative Tafel plots by taking a screenshot of their outcomes (some examples of those reports are provided in the Supporting Information).

## 8. CONCLUSION

We designed an interactive web interface for performing FOWA. This web application can successfully generate FOWA traces using the users' provided raw CV data and required parameters. The users will also get access to select the segments of those FOWA traces to perform a linear fitting that would consequently provide the reaction rate constant. Furthermore, we have also built up a library of the electrocatalysts for multielectron and multiproton reactions, mainly for $CO_2$RR and the web tools can compile the reported *TOF* and $\eta$ values for those catalysts to construct the catalytic Tafel plots. Overall, we believe that such a web-based interface will provide a concise guideline to perform kinetic analysis for the nonideal and ideal catalytic CVs and reduce the common errors that may occur while performing the FOWA using manually operated plotting applications.

## ■ ASSOCIATED CONTENT

### Supporting Information

The Supporting Information is available at https://pubs.acs.org/doi/10.1021/acs.jchemed.4c00932.

Examples of teaching modules and students report (PDF)

Raw data used to construct the FOWA traces presented in this manuscript (XLS)

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### Notes

The authors declare no competing financial interest.

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