New Electrochemical Simulation Features in AfterMath Electrochemical Studio

The new electrochemical simulation component of AfterMath Electrochemical Studio is an exciting and highly requested feature. Our goal is to provide an integrated solution into our already powerful AfterMath Electrochemical Studio software application. There are inherent benefits in only having to use one single application to acquire experimental data, fit those data, analyze, and plot, and now simulate. By integrating these components into a single application, it saves time and hassle as users do not have to import/export across more than one application.

Other electrochemical simulation software exists at various price points and capabilities. Some of these options might be free but lack in features or flexibility and have little to no support. Others might be full featured, yet costly, and are not well-developed or user-friendly for a broad audience, like newcomers to electrochemistry. A team of Pine Research electrochemical scientists and software engineers actively support AfterMath Electrochemical Studio.

Over time, you can expect new features and capabilities to be added by our team and we are open to your input as to what additional features you would like to see.

About our simulation engine

The electrochemical simulation engine employs fast quasi-explicit finite difference (FQEFD) for semi-infinite linear diffusion[1–3] utilizing an exponentially expanding space grid (based on the DuFort-Frankel algorithm). This method has been found to give highly accurate results as compared to theory. It is particularly effective for dealing with mathematically stiff problems, which involve large values of one or more homogenous rate constants and/or a wide dynamic range of homogenous rate constants. The FQEFD method enhances the computational speed by several orders of magnitude as compared to the traditional fast implicit finite difference (FIFD) method.

Confidence in our output

In using any new software, users might be skeptical or uncertain about what the software reports. We have found it very helpful to compare the output from our simulation software to the classic examples found in the 2nd Edition of Electrochemical Methods by Bard and Faulkner[4]. We simulated the following examples in AfterMath Electrochemical Studio. The plots were customized (colors, weights, fonts, etc.) in AfterMath to resemble the examples in the text. In all cases, the output from our simulations exactly matches the cases provided in the text.

Figure 12.3.2 Cyclic voltammograms for C_rE_r case

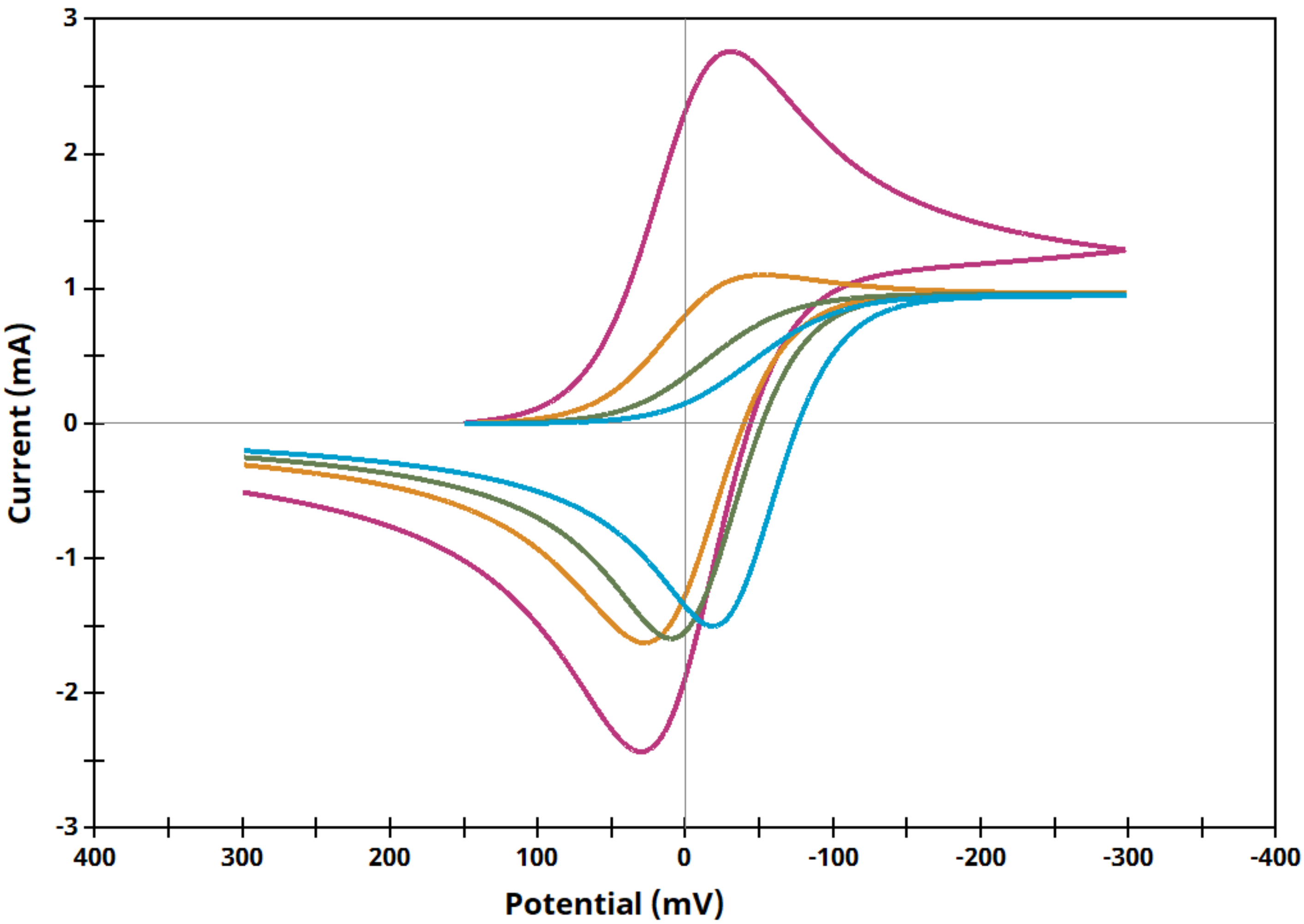


Figure 12.3.10 Cyclic voltammograms for E_rC_i case

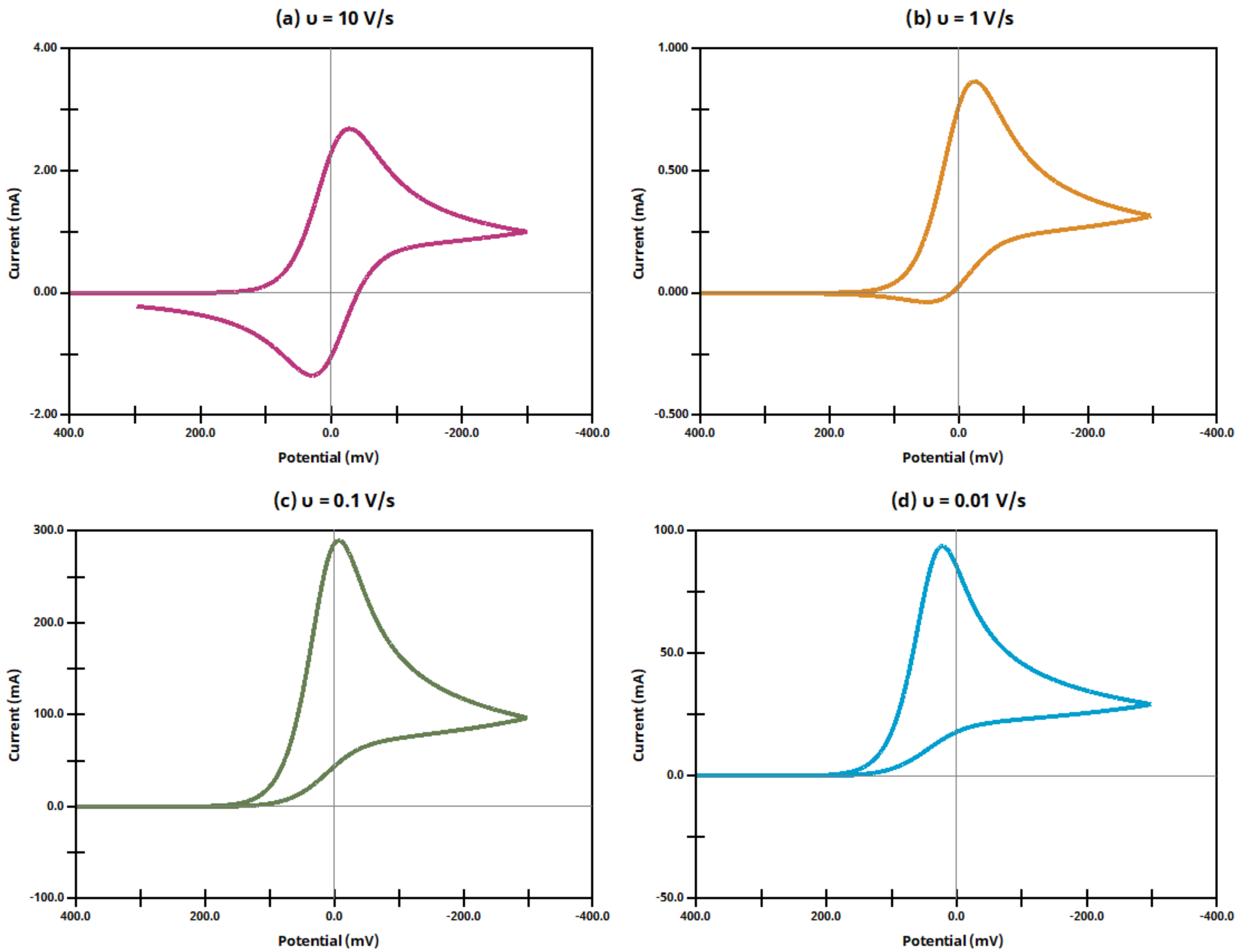


Figure 12.3.17 Cyclic voltammograms for E_rC_i' case

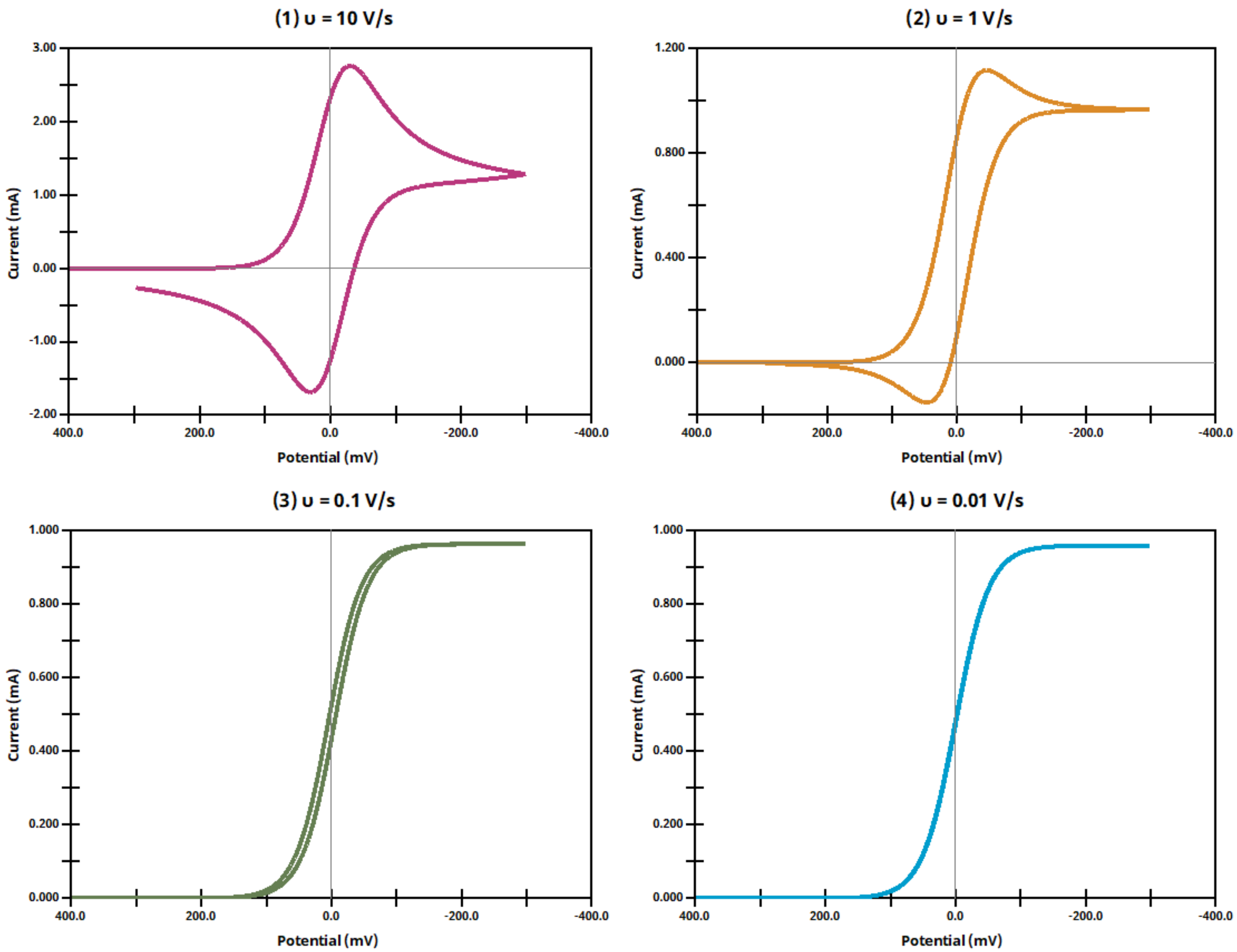


Figure 12.3.24 Cyclic voltammograms for E_rE_r case

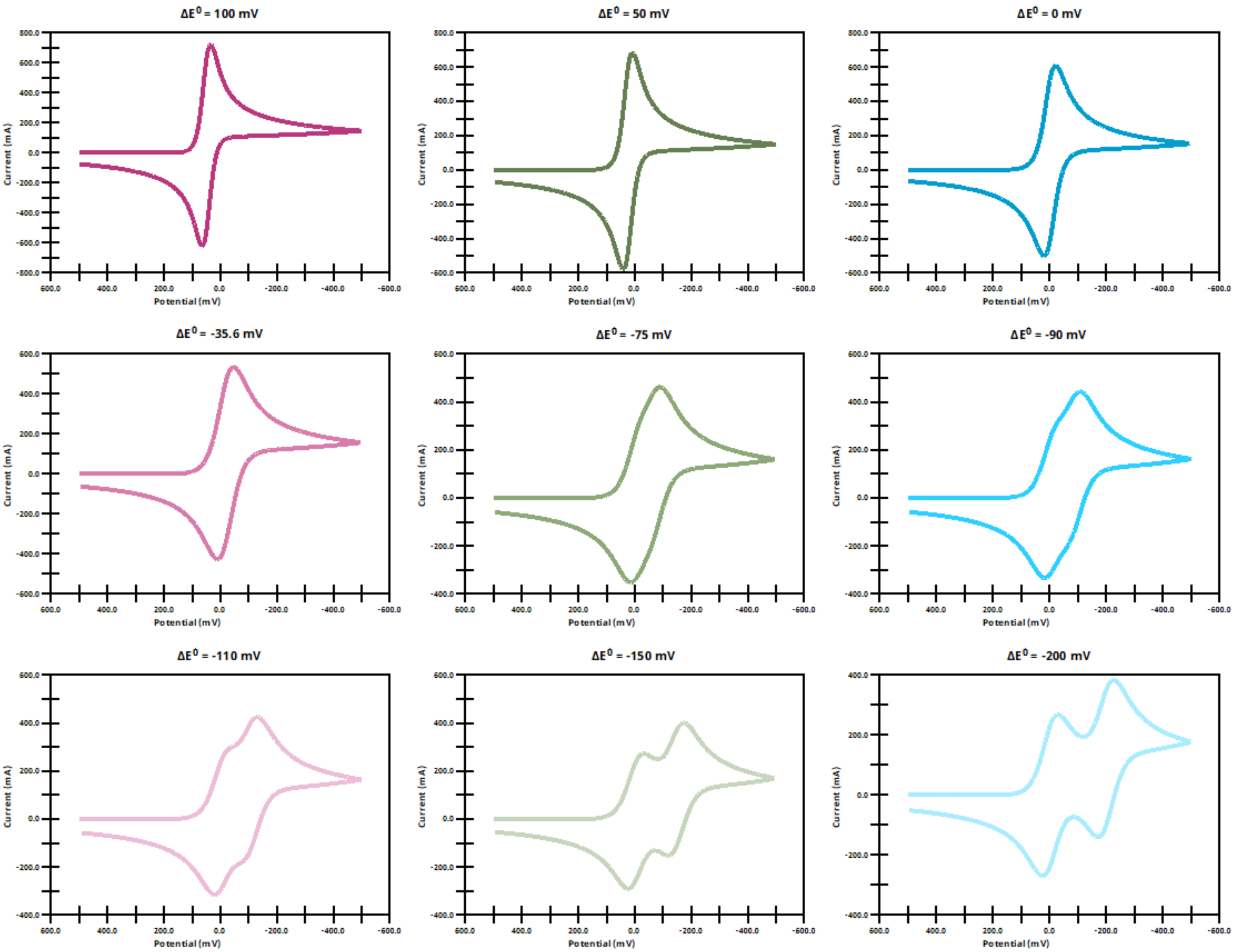


Figure 12.3.28 Cyclic voltammograms for E_rE_q case

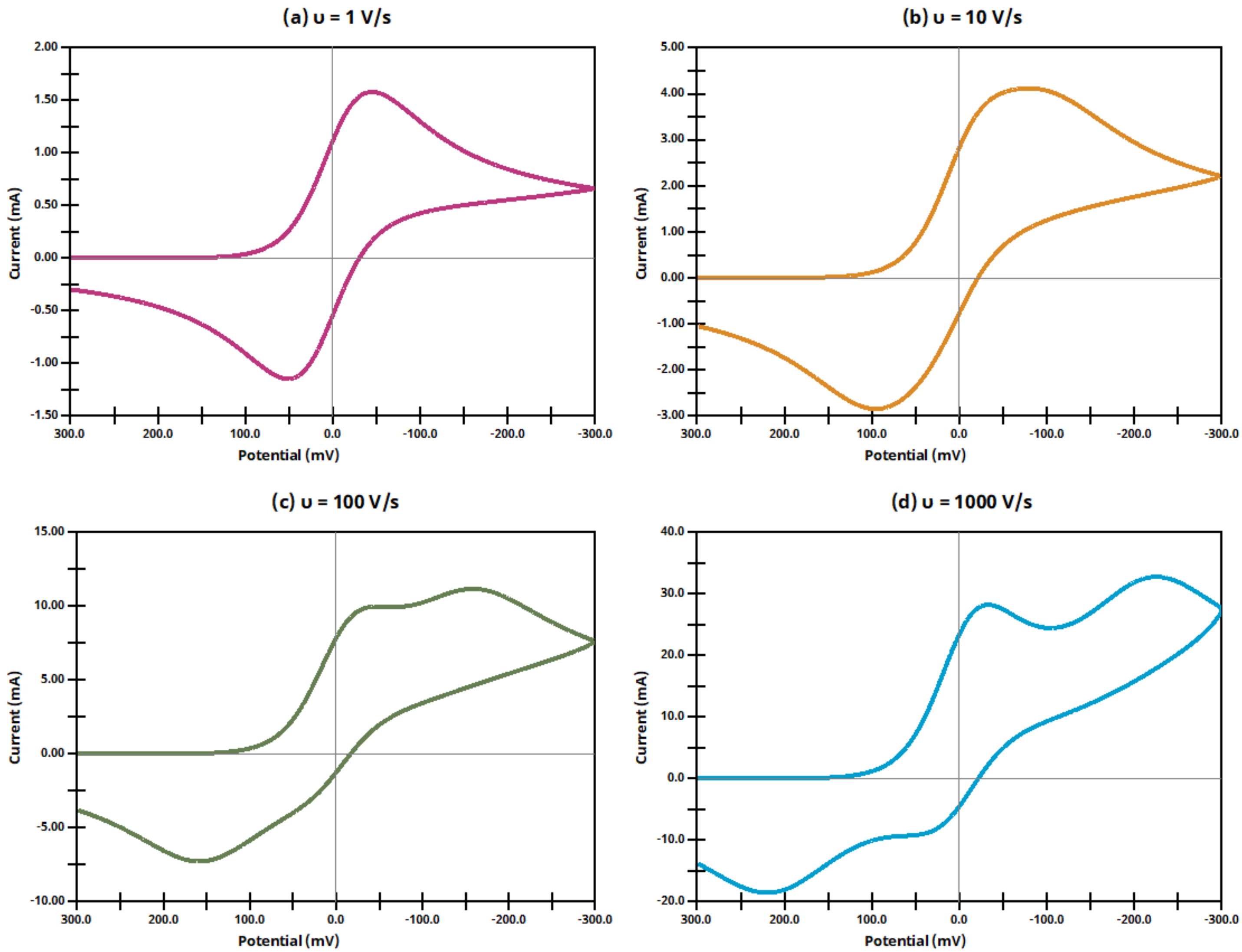
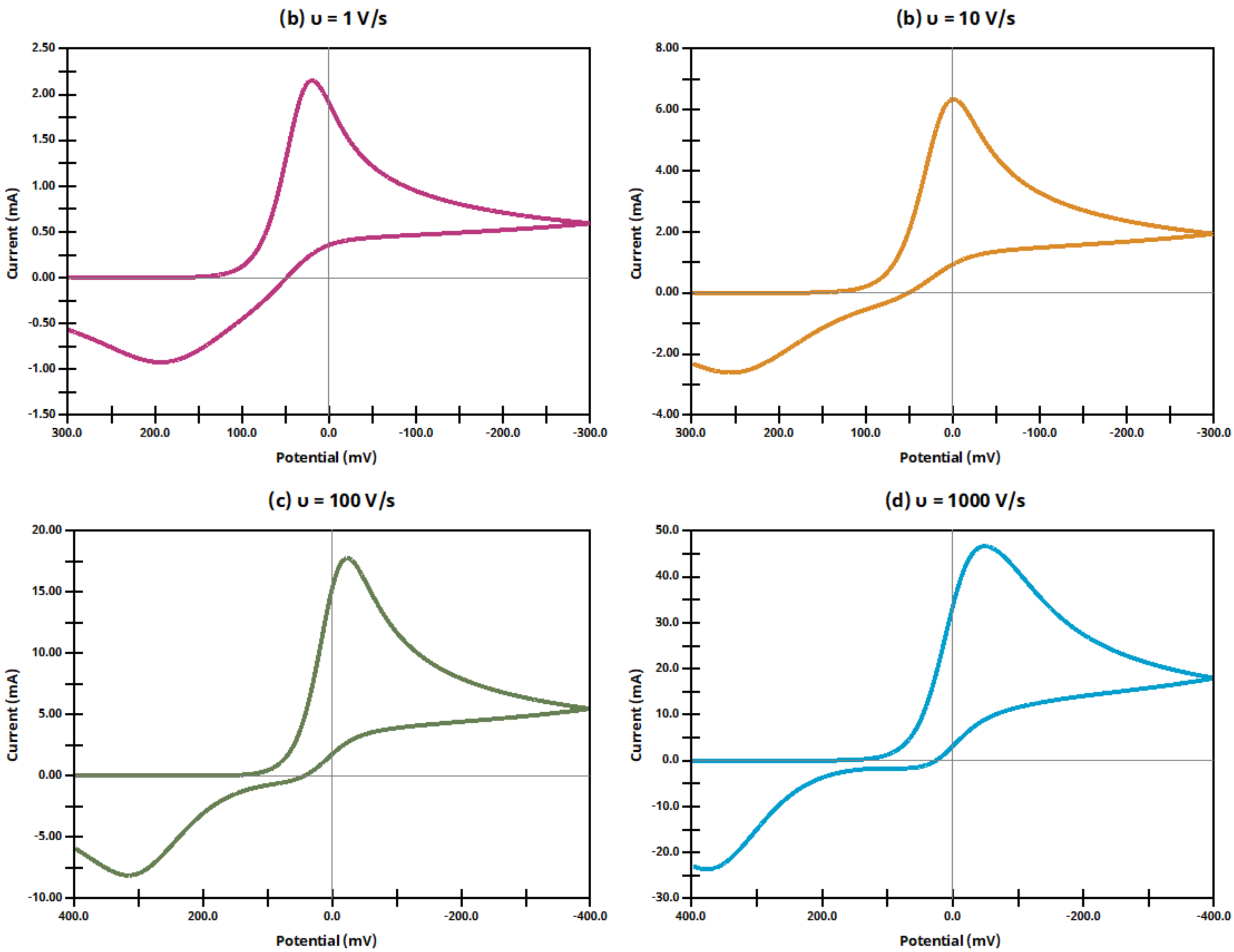


Figure 12.3.29 Cyclic voltammograms for E_rE_q case, ΔE^0 = 150 mV*



**In the second edition of Bard and Faulkner's Electrochemical Methods, figures 12.3.29 (a) and 12.3.29 (b) were erroneously duplicated from an adjacent figure. These figures will be updated appropriately in the third edition of the book.*

Figure 12.3.30 Cyclic voltammograms for E_qE_r case

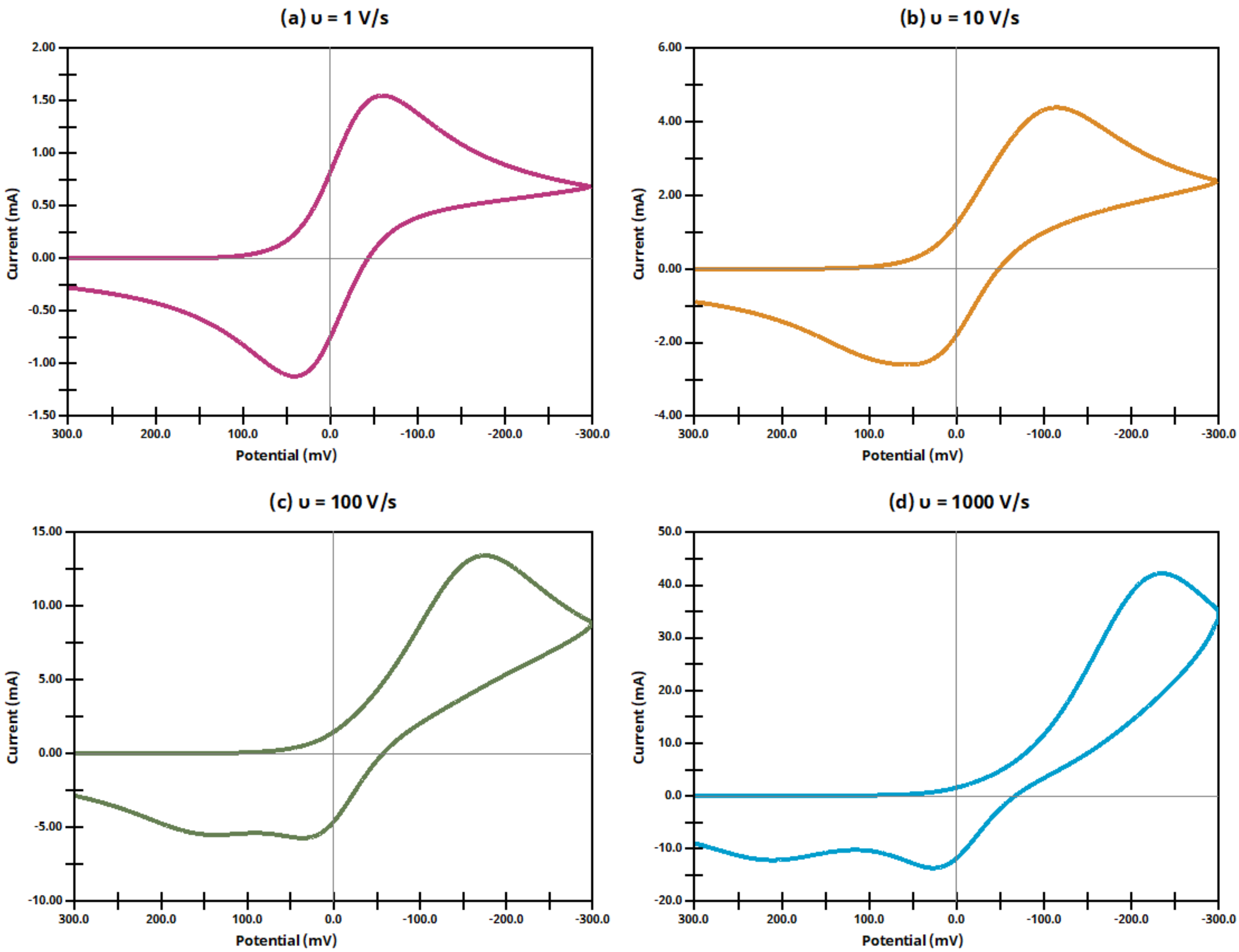
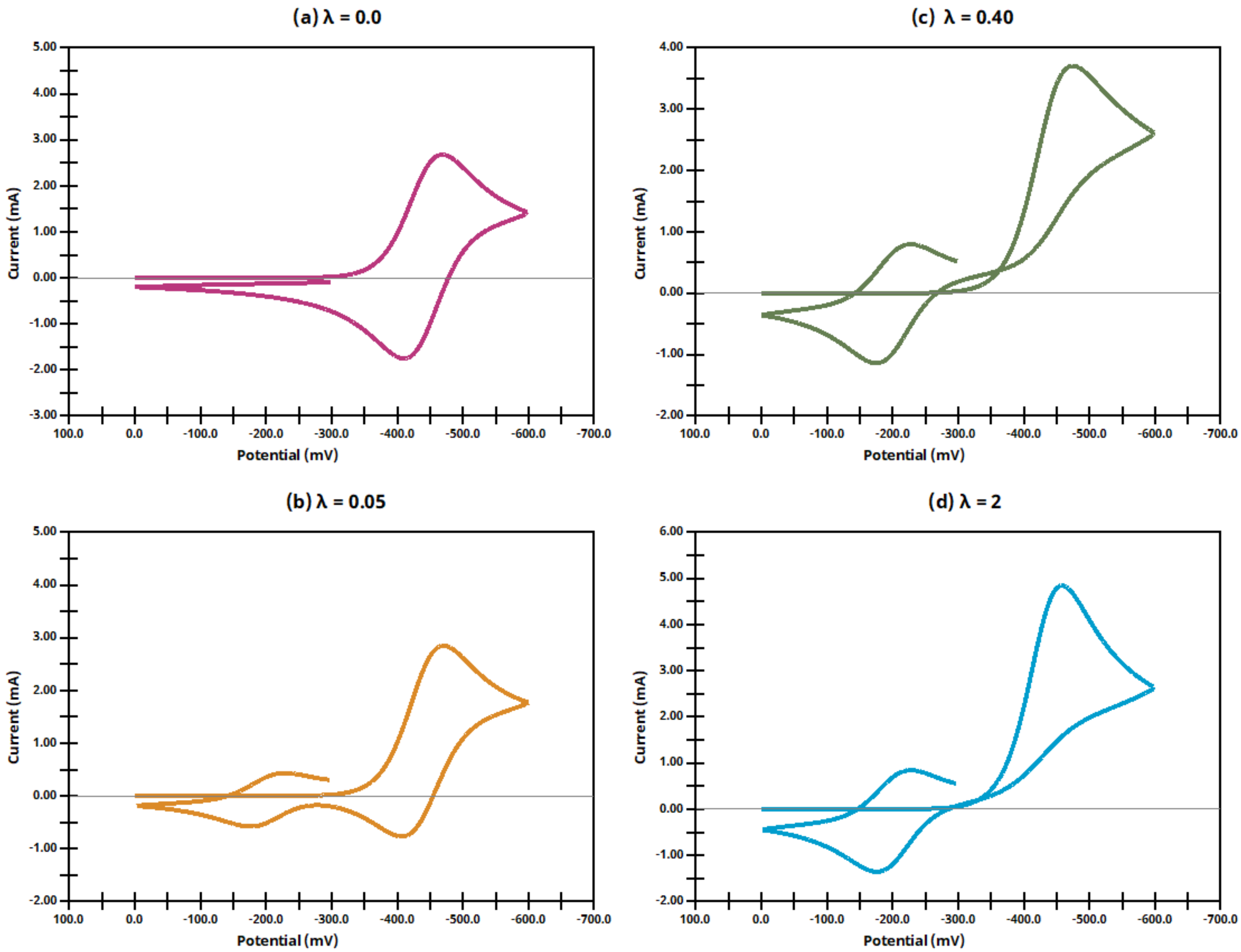


Figure 12.3.30 Cyclic voltammograms for $E_rC_iE_r$ case



References

(1) Rudolph, M. A Fast Implicit Finite Difference Algorithm for the Digital Simulation of Electrochemical Processes. *J. Electroanal. Chem. Interfacial Electrochem.* **1991**, *314* (1), 13–22. https://doi.org/10.1016/0022-0728(91)85425-O.

(2) Feldberg, S. W. A Fast Quasi-Explicit Finite Difference Method for Simulating Electrochemical Phenomena: Part I. Application to Cyclic Voltammetric Problems. *J. Electroanal. Chem. Interfacial Electrochem.* **1990**, *290* (1), 49–65. https://doi.org/10.1016/0022-0728(90)87419-K.

(3) Feldberg, S. W. Optimization of Explicit Finite-Difference Simulation of Electrochemical Phenomena Utilizing an Exponentially Expanded Space Grid: Refinement of the Joslin-Pletcher Algorithm. *J. Electroanal. Chem. Interfacial Electrochem.* **1981**, *127* (1), 1–10. https://doi.org/10.1016/S0022-0728(81)80462-7.

(4) Bard, A. J.; Faulkner, L. R. *Electrochemical Methods Fundamentals and Applications*, 2nd ed.; John Wiley & Sons, Inc.: New York, 2001.