The use of digital simulation to improve the cyclic voltammetric determination of rate constants for homogeneous chemical reactions following charge transfers

Carbajo, J.

Mozo, J. D.

Sturm, J. C.

Núñez-Vergara, L. J.

Moscoso, R.

Squella, J. A.

Cyclic voltammetry (CV) is a very useful electrochemical tool used to study reaction systems that include chemical steps that are coupled to electron transfers. This type of system generally involves the chemical reaction of an electrochemically generated free radical. Published methods exist that are used to determine the kinetics of electrochemically initiated chemical reactions from the measurements of the peak current ratio (ipa/ipc) of a cyclic voltammogram. The published method requires working curves to relate a kinetic parameter to the peak current ratio. In the presented work, a digital simulation package was used to obtain improved working curves for specific working conditions. The curves were compared with the published results for the first- and second-order chemical reactions following the charge transfer step mechanisms. According to the presented results, the previously published working curve is reliable for a mechanism with a first-order chemical reaction; however, a ch