Área: ELE

An adaptative mesh model for digital simulations of cyclic voltammetry

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Highlights

A static two-dimensional adaptive mesh model was optimized to simulate a cyclic voltammetry experiment using the finite element method (FEM) on MATLAB. The scan rate was the main parameter considered.

Abstract

The finite element method (FEM) may be applied to electrochemical simulations by solving Fick's laws on partial differential equations (PDEs) software.[1,2] An effective algorithm must adequately describe the electrode's surroundings to yield rapid and precise results.[3] Such geometric aspects are determined by a computational grid of discretized points in space, a mesh, for which an approximate solution to the system is calculated. This study optimizes the mesh generation script, a critical time-consuming step on FEM, of a cyclic voltammetry simulation using MATLAB's PDE Toolbox. An adaptative model is presented for a triangular mesh that varies according to the scan rate established in the simulation, due to its influence on the growth of the diffusion layer at vicinity of the electrode. The proposed model has been calibrated for macroelectrodes by comparing the simulated results for reversible voltammograms with theoretical predictions given by Randles–Ševčík equation, namely the anodic peak current and peak to peak separation. Mesh generation conditions were altered to determine optimal script parameters for different scan rates. The mesh's parameters were then adjusted to properly fit the obtained data and modulate the simulation's geometry, ensuring stable, accurate and faster outcomes.

References:

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