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A Systematic Strategy for Optimizing Heterogeneous Catalysis using Finite Element Method Simulations via Adaptive Mesh Refinement Algorithms

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Finite element method (FEM) simulations are used to model electrochemical systems by solving Fick's laws of diffusion and to aid the interpretation of experimental data based on theoretical predictions [1]. Although commercially available software can solve general problems, complex systems require tailor-made scripts that adequately describe their geometry and boundary conditions. In FEM programs, the computed domain is defined by a predetermined arrangement of points in space, a mesh, which determines the precision and time of a simulation [2]. Thus, scripts created for more specific purposes require a fine meshing adjustment to become effective. In this work, a generic algorithm for the creation of an adaptive mesh model is developed and applied to a MATLAB heterogeneous catalysis cyclic voltammetry simulation. The studied system considers the Nernstian electrochemical reaction of an oxidized catalyst adsorbed on the surface of a circular electrode and a bimolecular chemical reaction of the reduced catalyst with a substrate in solution. Different meshes were tested for various experimental conditions and compared with high resolution FEM simulations. The optimization algorithm applies a multiparametric fit of ideal mesh generation parameters with an extension of Taylor polynomials for multivariable functions. The resulting adaptive mesh model adjusted the mesh's geometry according to the obtained data to ensure stable, accurate, and faster outcomes.

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